Entering Gaussian System, Link 0=g09

Initial command:

/apps/gaussian/g09d01/g09/l1.exe "/srv/scratch/z5105842/Gau-48195.inp" -scrdir="/srv/scratch/z5105842/"

Entering Link 1 = /apps/gaussian/g09d01/g09/l1.exe PID= 48196.

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---------------------------------------------------------------

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Cite this work as:

Gaussian 09, Revision D.01,

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,

M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci,

G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian,

A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada,

M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima,

Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr.,

J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers,

K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand,

K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi,

M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross,

V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,

O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,

R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth,

P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels,

O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski,

and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Gaussian 09: ES64L-G09RevD.01 24-Apr-2013

17-Aug-2019

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

%nprocshared=12

Will use up to 12 processors via shared memory.

%chk=BTPAanion.chk

%mem=10GB

----------------------------------------------------------------------

#p opt b3lyp/6-311g\* scrf=(solvent=dmso,smd) empiricaldispersion=gd3bj

----------------------------------------------------------------------

1/14=-1,18=20,19=15,26=3,38=1/1,3;

2/9=110,12=2,17=6,18=5,40=1/2;

3/5=4,6=6,7=1,11=2,16=1,25=1,30=1,70=32201,71=1,72=21,74=-5,124=41/1,2,3;

4//1;

5/5=2,38=5,53=21/2;

6/7=2,8=2,9=2,10=2,28=1/1;

7//1,2,3,16;

1/14=-1,18=20,19=15,26=3/3(2);

2/9=110/2;

99//99;

2/9=110/2;

3/5=4,6=6,7=1,11=2,16=1,25=1,30=1,70=32205,71=1,72=21,74=-5,124=41/1,2,3;

4/5=5,16=3,69=1/1;

5/5=2,38=5,53=21/2;

7//1,2,3,16;

1/14=-1,18=20,19=15,26=3/3(-5);

2/9=110/2;

6/7=2,8=2,9=2,10=2,19=2,28=1/1;

99/9=1/99;

Leave Link 1 at Sat Aug 17 17:28:22 2019, MaxMem= 1342177280 cpu: 0.9

(Enter /apps/gaussian/g09d01/g09/l101.exe)

---------

BTPAanion

---------

Symbolic Z-matrix:

Charge = -1 Multiplicity = 2

C -4.15048 -0.29878 -0.10318

C -2.80051 0.00247 0.47953

O -4.92542 0.53895 -0.53826

O -4.43537 -1.62131 -0.14719

C -2.3553 -0.91805 1.60567

S -1.57205 -0.01868 -0.97653

C -0.10996 0.6342 -0.2421

S 1.13146 -0.62662 0.0574

S -0.02308 2.23096 0.39902

C 2.70798 0.30503 -0.10326

C 3.89819 -0.64851 -0.01424

C 5.23655 0.09195 -0.1254

C 6.43923 -0.85161 -0.05712

H -2.81503 1.04432 0.80514

H -5.31113 -1.71998 -0.5651

H -1.38108 -0.59086 1.97816

H -3.0689 -0.87328 2.43746

H -2.27036 -1.95485 1.27185

H 2.69378 0.82462 -1.06705

H 2.7478 1.05747 0.68824

H 3.86571 -1.19484 0.93804

H 3.83267 -1.39931 -0.81271

H 5.26126 0.65126 -1.07026

H 5.30658 0.83593 0.67933

H 7.38318 -0.3016 -0.14535

H 6.45941 -1.39827 0.89367

H 6.40705 -1.59221 -0.86553

NAtoms= 27 NQM= 27 NQMF= 0 NMMI= 0 NMMIF= 0

NMic= 0 NMicF= 0.

Isotopes and Nuclear Properties:

(Nuclear quadrupole moments (NQMom) in fm\*\*2, nuclear magnetic moments (NMagM)

in nuclear magnetons)

Atom 1 2 3 4 5 6 7 8 9 10

IAtWgt= 12 12 16 16 12 32 12 32 32 12

AtmWgt= 12.0000000 12.0000000 15.9949146 15.9949146 12.0000000 31.9720718 12.0000000 31.9720718 31.9720718 12.0000000

NucSpn= 0 0 0 0 0 0 0 0 0 0

AtZEff= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NMagM= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

AtZNuc= 6.0000000 6.0000000 8.0000000 8.0000000 6.0000000 16.0000000 6.0000000 16.0000000 16.0000000 6.0000000

Atom 11 12 13 14 15 16 17 18 19 20

IAtWgt= 12 12 12 1 1 1 1 1 1 1

AtmWgt= 12.0000000 12.0000000 12.0000000 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250

NucSpn= 0 0 0 1 1 1 1 1 1 1

AtZEff= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NMagM= 0.0000000 0.0000000 0.0000000 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460

AtZNuc= 6.0000000 6.0000000 6.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000

Atom 21 22 23 24 25 26 27

IAtWgt= 1 1 1 1 1 1 1

AtmWgt= 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250

NucSpn= 1 1 1 1 1 1 1

AtZEff= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NMagM= 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460

AtZNuc= 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000

Leave Link 101 at Sat Aug 17 17:28:22 2019, MaxMem= 1342177280 cpu: 2.9

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Initialization pass.

----------------------------

! Initial Parameters !

! (Angstroms and Degrees) !

-------------------------- --------------------------

! Name Definition Value Derivative Info. !

--------------------------------------------------------------------------------

! R1 R(1,2) 1.5009 estimate D2E/DX2 !

! R2 R(1,3) 1.2213 estimate D2E/DX2 !

! R3 R(1,4) 1.3536 estimate D2E/DX2 !

! R4 R(2,5) 1.5211 estimate D2E/DX2 !

! R5 R(2,6) 1.9052 estimate D2E/DX2 !

! R6 R(2,14) 1.0916 estimate D2E/DX2 !

! R7 R(4,15) 0.9754 estimate D2E/DX2 !

! R8 R(5,16) 1.0931 estimate D2E/DX2 !

! R9 R(5,17) 1.0969 estimate D2E/DX2 !

! R10 R(5,18) 1.0925 estimate D2E/DX2 !

! R11 R(6,7) 1.7616 estimate D2E/DX2 !

! R12 R(7,8) 1.7946 estimate D2E/DX2 !

! R13 R(7,9) 1.7228 estimate D2E/DX2 !

! R14 R(8,10) 1.8383 estimate D2E/DX2 !

! R15 R(10,11) 1.5277 estimate D2E/DX2 !

! R16 R(10,19) 1.095 estimate D2E/DX2 !

! R17 R(10,20) 1.0928 estimate D2E/DX2 !

! R18 R(11,12) 1.5336 estimate D2E/DX2 !

! R19 R(11,21) 1.0983 estimate D2E/DX2 !

! R20 R(11,22) 1.098 estimate D2E/DX2 !

! R21 R(12,13) 1.5302 estimate D2E/DX2 !

! R22 R(12,23) 1.0983 estimate D2E/DX2 !

! R23 R(12,24) 1.0982 estimate D2E/DX2 !

! R24 R(13,25) 1.0961 estimate D2E/DX2 !

! R25 R(13,26) 1.0969 estimate D2E/DX2 !

! R26 R(13,27) 1.0968 estimate D2E/DX2 !

! A1 A(2,1,3) 124.8434 estimate D2E/DX2 !

! A2 A(2,1,4) 113.4549 estimate D2E/DX2 !

! A3 A(3,1,4) 121.6726 estimate D2E/DX2 !

! A4 A(1,2,5) 115.4183 estimate D2E/DX2 !

! A5 A(1,2,6) 106.3207 estimate D2E/DX2 !

! A6 A(1,2,14) 107.181 estimate D2E/DX2 !

! A7 A(5,2,6) 111.7389 estimate D2E/DX2 !

! A8 A(5,2,14) 111.1393 estimate D2E/DX2 !

! A9 A(6,2,14) 104.3074 estimate D2E/DX2 !

! A10 A(1,4,15) 107.5622 estimate D2E/DX2 !

! A11 A(2,5,16) 109.3901 estimate D2E/DX2 !

! A12 A(2,5,17) 110.2615 estimate D2E/DX2 !

! A13 A(2,5,18) 111.7674 estimate D2E/DX2 !

! A14 A(16,5,17) 108.0107 estimate D2E/DX2 !

! A15 A(16,5,18) 108.5953 estimate D2E/DX2 !

! A16 A(17,5,18) 108.7252 estimate D2E/DX2 !

! A17 A(2,6,7) 102.2644 estimate D2E/DX2 !

! A18 A(6,7,8) 112.5401 estimate D2E/DX2 !

! A19 A(6,7,9) 122.7165 estimate D2E/DX2 !

! A20 A(8,7,9) 123.6534 estimate D2E/DX2 !

! A21 A(7,8,10) 102.8622 estimate D2E/DX2 !

! A22 A(8,10,11) 110.2881 estimate D2E/DX2 !

! A23 A(8,10,19) 107.8355 estimate D2E/DX2 !

! A24 A(8,10,20) 108.4764 estimate D2E/DX2 !

! A25 A(11,10,19) 110.9506 estimate D2E/DX2 !

! A26 A(11,10,20) 111.0498 estimate D2E/DX2 !

! A27 A(19,10,20) 108.1337 estimate D2E/DX2 !

! A28 A(10,11,12) 111.983 estimate D2E/DX2 !

! A29 A(10,11,21) 109.7521 estimate D2E/DX2 !

! A30 A(10,11,22) 109.7518 estimate D2E/DX2 !

! A31 A(12,11,21) 109.1977 estimate D2E/DX2 !

! A32 A(12,11,22) 109.2399 estimate D2E/DX2 !

! A33 A(21,11,22) 106.775 estimate D2E/DX2 !

! A34 A(11,12,13) 112.6413 estimate D2E/DX2 !

! A35 A(11,12,23) 109.1406 estimate D2E/DX2 !

! A36 A(11,12,24) 109.2466 estimate D2E/DX2 !

! A37 A(13,12,23) 109.5567 estimate D2E/DX2 !

! A38 A(13,12,24) 109.5684 estimate D2E/DX2 !

! A39 A(23,12,24) 106.4982 estimate D2E/DX2 !

! A40 A(12,13,25) 111.3385 estimate D2E/DX2 !

! A41 A(12,13,26) 111.1276 estimate D2E/DX2 !

! A42 A(12,13,27) 111.1258 estimate D2E/DX2 !

! A43 A(25,13,26) 107.6985 estimate D2E/DX2 !

! A44 A(25,13,27) 107.7437 estimate D2E/DX2 !

! A45 A(26,13,27) 107.6316 estimate D2E/DX2 !

! D1 D(3,1,2,5) 146.6661 estimate D2E/DX2 !

! D2 D(3,1,2,6) -88.8313 estimate D2E/DX2 !

! D3 D(3,1,2,14) 22.2727 estimate D2E/DX2 !

! D4 D(4,1,2,5) -35.273 estimate D2E/DX2 !

! D5 D(4,1,2,6) 89.2296 estimate D2E/DX2 !

! D6 D(4,1,2,14) -159.6664 estimate D2E/DX2 !

! D7 D(2,1,4,15) -178.0997 estimate D2E/DX2 !

! D8 D(3,1,4,15) 0.0304 estimate D2E/DX2 !

! D9 D(1,2,5,16) -178.0512 estimate D2E/DX2 !

! D10 D(1,2,5,17) -59.4094 estimate D2E/DX2 !

! D11 D(1,2,5,18) 61.6472 estimate D2E/DX2 !

! D12 D(6,2,5,16) 60.3181 estimate D2E/DX2 !

! D13 D(6,2,5,17) 178.9599 estimate D2E/DX2 !

! D14 D(6,2,5,18) -59.9835 estimate D2E/DX2 !

! D15 D(14,2,5,16) -55.7483 estimate D2E/DX2 !

! D16 D(14,2,5,17) 62.8936 estimate D2E/DX2 !

! D17 D(14,2,5,18) -176.0499 estimate D2E/DX2 !

! D18 D(1,2,6,7) 169.8237 estimate D2E/DX2 !

! D19 D(5,2,6,7) -63.4321 estimate D2E/DX2 !

! D20 D(14,2,6,7) 56.7245 estimate D2E/DX2 !

! D21 D(2,6,7,8) 105.7426 estimate D2E/DX2 !

! D22 D(2,6,7,9) -62.7074 estimate D2E/DX2 !

! D23 D(6,7,8,10) 149.7529 estimate D2E/DX2 !

! D24 D(9,7,8,10) -41.9231 estimate D2E/DX2 !

! D25 D(7,8,10,11) -174.3773 estimate D2E/DX2 !

! D26 D(7,8,10,19) -53.0852 estimate D2E/DX2 !

! D27 D(7,8,10,20) 63.8015 estimate D2E/DX2 !

! D28 D(8,10,11,12) -179.2482 estimate D2E/DX2 !

! D29 D(8,10,11,21) -57.7997 estimate D2E/DX2 !

! D30 D(8,10,11,22) 59.2499 estimate D2E/DX2 !

! D31 D(19,10,11,12) 61.3323 estimate D2E/DX2 !

! D32 D(19,10,11,21) -177.2192 estimate D2E/DX2 !

! D33 D(19,10,11,22) -60.1696 estimate D2E/DX2 !

! D34 D(20,10,11,12) -58.9627 estimate D2E/DX2 !

! D35 D(20,10,11,21) 62.4858 estimate D2E/DX2 !

! D36 D(20,10,11,22) 179.5354 estimate D2E/DX2 !

! D37 D(10,11,12,13) -179.2206 estimate D2E/DX2 !

! D38 D(10,11,12,23) -57.3042 estimate D2E/DX2 !

! D39 D(10,11,12,24) 58.7729 estimate D2E/DX2 !

! D40 D(21,11,12,13) 59.0123 estimate D2E/DX2 !

! D41 D(21,11,12,23) -179.0713 estimate D2E/DX2 !

! D42 D(21,11,12,24) -62.9942 estimate D2E/DX2 !

! D43 D(22,11,12,13) -57.4248 estimate D2E/DX2 !

! D44 D(22,11,12,23) 64.4917 estimate D2E/DX2 !

! D45 D(22,11,12,24) -179.4312 estimate D2E/DX2 !

! D46 D(11,12,13,25) 179.6137 estimate D2E/DX2 !

! D47 D(11,12,13,26) -60.3293 estimate D2E/DX2 !

! D48 D(11,12,13,27) 59.5007 estimate D2E/DX2 !

! D49 D(23,12,13,25) 57.9329 estimate D2E/DX2 !

! D50 D(23,12,13,26) 177.99 estimate D2E/DX2 !

! D51 D(23,12,13,27) -62.1801 estimate D2E/DX2 !

! D52 D(24,12,13,25) -58.5619 estimate D2E/DX2 !

! D53 D(24,12,13,26) 61.4952 estimate D2E/DX2 !

! D54 D(24,12,13,27) -178.6749 estimate D2E/DX2 !

--------------------------------------------------------------------------------

Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06

Number of steps in this run= 135 maximum allowed number of steps= 162.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:28:22 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.150485 -0.298780 -0.103181

2 6 0 -2.800509 0.002466 0.479533

3 8 0 -4.925424 0.538952 -0.538258

4 8 0 -4.435366 -1.621313 -0.147193

5 6 0 -2.355300 -0.918051 1.605670

6 16 0 -1.572047 -0.018680 -0.976528

7 6 0 -0.109960 0.634201 -0.242097

8 16 0 1.131455 -0.626624 0.057400

9 16 0 -0.023079 2.230955 0.399021

10 6 0 2.707977 0.305025 -0.103256

11 6 0 3.898192 -0.648513 -0.014237

12 6 0 5.236548 0.091947 -0.125404

13 6 0 6.439227 -0.851612 -0.057122

14 1 0 -2.815027 1.044322 0.805135

15 1 0 -5.311130 -1.719979 -0.565097

16 1 0 -1.381081 -0.590863 1.978162

17 1 0 -3.068902 -0.873278 2.437455

18 1 0 -2.270360 -1.954853 1.271845

19 1 0 2.693780 0.824615 -1.067048

20 1 0 2.747799 1.057468 0.688237

21 1 0 3.865705 -1.194843 0.938040

22 1 0 3.832672 -1.399309 -0.812709

23 1 0 5.261256 0.651255 -1.070263

24 1 0 5.306577 0.835932 0.679334

25 1 0 7.383178 -0.301600 -0.145354

26 1 0 6.459411 -1.398272 0.893670

27 1 0 6.407053 -1.592205 -0.865532

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.500913 0.000000

3 O 1.221318 2.416398 0.000000

4 O 1.353583 2.387928 2.249407 0.000000

5 C 2.554674 1.521101 3.650318 2.809587 0.000000

6 S 2.736701 1.905172 3.427561 3.384498 2.844310

7 C 4.149168 2.856378 4.825503 4.879087 3.296253

8 S 5.294540 4.004284 6.196706 5.658689 3.826164

9 S 4.866955 3.561848 5.270138 5.882737 4.100182

10 C 6.884990 5.547486 7.649363 7.398652 5.482072

11 C 8.056763 6.748346 8.918569 8.391198 6.465517

12 C 9.395188 8.060288 10.180174 9.822508 7.851934

13 C 10.604232 9.294631 11.459514 10.902171 8.950586

14 H 2.100573 1.091646 2.552230 3.261600 2.168666

15 H 1.892160 3.218895 2.291781 0.975367 3.753964

16 H 3.476622 2.147721 4.491238 3.861038 1.093117

17 H 2.820408 2.161578 3.780997 3.017811 1.096859

18 H 2.857997 2.177134 4.067542 2.610013 1.092526

19 H 7.002501 5.766719 7.642872 7.592985 5.972731

20 H 7.074749 5.651576 7.787907 7.711788 5.548511

21 H 8.133042 6.788386 9.081269 8.382564 6.262847

22 H 8.089832 6.901735 8.974209 8.297750 6.661168

23 H 9.508874 8.234977 10.201181 10.002055 8.224066

24 H 9.556983 8.152265 10.308471 10.081005 7.914475

25 H 11.533740 10.207371 12.343524 11.891998 9.913831

26 H 10.713192 9.374417 11.636912 10.946657 8.856449

27 H 10.663758 9.440941 11.535769 10.866228 9.129083

6 7 8 9 10

6 S 0.000000

7 C 1.761630 0.000000

8 S 2.957622 1.794572 0.000000

9 S 3.058152 1.722848 3.100873 0.000000

10 C 4.380182 2.840493 1.838261 3.379372 0.000000

11 C 5.589831 4.214565 2.767751 4.882467 1.527668

12 C 6.862479 5.375203 4.171517 5.702110 2.537630

13 C 8.106762 6.718162 5.313773 7.174377 3.906682

14 H 2.418532 2.929553 4.350389 3.060719 5.645822

15 H 4.128491 5.718274 6.564284 6.671048 8.283720

16 H 3.015635 2.836561 3.162822 3.507209 4.674966

17 H 3.824421 4.267063 4.834098 4.802969 6.419964

18 H 3.048211 3.696289 3.848560 4.830433 5.637534

19 H 4.349324 2.928781 2.410672 3.392414 1.095021

20 H 4.752958 3.035039 2.417993 3.022992 1.092803

21 H 5.883713 4.532553 2.928229 5.210497 2.161998

22 H 5.580677 4.472707 2.941208 5.432672 2.161716

23 H 6.866704 5.434714 4.467645 5.707753 2.752129

24 H 7.126550 5.498055 4.467384 5.516330 2.765327

25 H 8.998164 7.551967 6.263449 7.846198 4.714581

26 H 8.360935 6.969760 5.448110 7.445713 4.238908

27 H 8.133532 6.914985 5.442066 7.586979 4.226548

11 12 13 14 15

11 C 0.000000

12 C 1.533570 0.000000

13 C 2.549499 1.530164 0.000000

14 H 6.971683 8.160930 9.485740 0.000000

15 H 9.287793 10.711205 11.793345 3.968555 0.000000

16 H 5.643022 6.977409 8.085022 2.471037 4.815429

17 H 7.389297 8.745308 9.829949 2.531030 3.841849

18 H 6.435182 7.905401 8.879200 3.083753 3.560310

19 H 2.174655 2.808766 4.225880 5.822396 8.414600

20 H 2.174223 2.790719 4.222178 5.564070 8.615764

21 H 1.098346 2.160082 2.780498 7.047248 9.313941

22 H 1.097973 2.160347 2.768576 7.265030 9.152773

23 H 2.159290 1.098269 2.161638 8.300480 10.846810

24 H 2.160594 1.098190 2.161728 8.125251 10.991678

25 H 3.504664 2.182498 1.096057 10.330456 12.780197

26 H 2.818914 2.180518 1.096928 9.591105 11.864954

27 H 2.812408 2.180422 1.096832 9.735973 11.722730

16 17 18 19 20

16 H 0.000000

17 H 1.771849 0.000000

18 H 1.774872 1.779360 0.000000

19 H 5.280282 6.955062 6.151305 0.000000

20 H 4.629098 6.373504 5.881887 1.771486 0.000000

21 H 5.382881 7.102142 6.191957 3.077661 2.526860

22 H 5.968732 7.646699 6.473098 2.511494 3.076612

23 H 7.413258 9.166233 8.306775 2.573324 3.094317

24 H 6.960422 8.727029 8.096266 3.142720 2.568366

25 H 9.022485 10.781637 9.896085 4.910024 4.901906

26 H 7.956214 9.666832 8.755667 4.792246 4.455213

27 H 8.351306 10.060830 8.944126 4.435090 4.777563

21 22 23 24 25

21 H 0.000000

22 H 1.762958 0.000000

23 H 3.064135 2.512369 0.000000

24 H 2.503415 3.065109 1.759900 0.000000

25 H 3.787379 3.775768 2.503186 2.507262 0.000000

26 H 2.602050 3.132330 3.081099 2.523219 1.770764

27 H 3.141531 2.582138 2.527425 3.081154 1.771197

26 27

26 H 0.000000

27 H 1.770634 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.150485 -0.298780 -0.103181

2 6 0 -2.800509 0.002466 0.479533

3 8 0 -4.925424 0.538952 -0.538258

4 8 0 -4.435366 -1.621313 -0.147193

5 6 0 -2.355300 -0.918051 1.605670

6 16 0 -1.572047 -0.018680 -0.976528

7 6 0 -0.109960 0.634201 -0.242097

8 16 0 1.131455 -0.626624 0.057400

9 16 0 -0.023079 2.230955 0.399021

10 6 0 2.707977 0.305025 -0.103256

11 6 0 3.898192 -0.648513 -0.014237

12 6 0 5.236548 0.091947 -0.125404

13 6 0 6.439227 -0.851612 -0.057122

14 1 0 -2.815027 1.044322 0.805135

15 1 0 -5.311130 -1.719979 -0.565097

16 1 0 -1.381081 -0.590863 1.978162

17 1 0 -3.068902 -0.873278 2.437455

18 1 0 -2.270360 -1.954853 1.271845

19 1 0 2.693780 0.824615 -1.067048

20 1 0 2.747799 1.057468 0.688237

21 1 0 3.865705 -1.194843 0.938040

22 1 0 3.832672 -1.399309 -0.812709

23 1 0 5.261256 0.651255 -1.070263

24 1 0 5.306577 0.835932 0.679334

25 1 0 7.383178 -0.301600 -0.145354

26 1 0 6.459411 -1.398272 0.893670

27 1 0 6.407053 -1.592205 -0.865532

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3904303 0.1892521 0.1776046

Leave Link 202 at Sat Aug 17 17:28:22 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1098.2270101612 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0545980748 Hartrees.

Nuclear repulsion after empirical dispersion term = 1098.1724120864 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2333

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.98D-08

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 96

GePol: Fraction of low-weight points (<1% of avg) = 4.11%

GePol: Cavity surface area = 311.233 Ang\*\*2

GePol: Cavity volume = 321.311 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057052661 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1098.1667068203 Hartrees.

Leave Link 301 at Sat Aug 17 17:28:22 2019, MaxMem= 1342177280 cpu: 0.8

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.88D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:28:23 2019, MaxMem= 1342177280 cpu: 2.8

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:28:23 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.62640129340

JPrj=0 DoOrth=F DoCkMO=F.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7500 S= 0.5000

Leave Link 401 at Sat Aug 17 17:28:23 2019, MaxMem= 1342177280 cpu: 6.4

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16328667.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.33D-15 for 2330.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.84D-15 for 718 121.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.55D-15 for 388.

Iteration 1 A^-1\*A deviation from orthogonality is 4.45D-10 for 887 884.

Iteration 2 A\*A^-1 deviation from unit magnitude is 9.21D-15 for 572.

Iteration 2 A\*A^-1 deviation from orthogonality is 3.30D-15 for 2296 19.

Iteration 2 A^-1\*A deviation from unit magnitude is 9.99D-16 for 2190.

Iteration 2 A^-1\*A deviation from orthogonality is 6.11D-16 for 2300 65.

E= -1658.22489885896

DIIS: error= 3.30D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.22489885896 IErMin= 1 ErrMin= 3.30D-02

ErrMax= 3.30D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.17D+00 BMatP= 2.17D+00

IDIUse=3 WtCom= 6.70D-01 WtEn= 3.30D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.112 Goal= None Shift= 0.000

Gap= 0.151 Goal= None Shift= 0.000

GapD= 0.112 DampG=1.000 DampE=0.500 DampFc=0.5000 IDamp=-1.

Damping current iteration by 5.00D-01

RMSDP=4.52D-03 MaxDP=2.43D-01 OVMax= 2.55D-01

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.25D-03 CP: 9.85D-01

E= -1658.38575532977 Delta-E= -0.160856470814 Rises=F Damp=T

DIIS: error= 8.62D-03 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.38575532977 IErMin= 2 ErrMin= 8.62D-03

ErrMax= 8.62D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.98D-01 BMatP= 2.17D+00

IDIUse=3 WtCom= 9.14D-01 WtEn= 8.62D-02

Coeff-Com: 0.142D+00 0.858D+00

Coeff-En: 0.267D+00 0.733D+00

Coeff: 0.153D+00 0.847D+00

Gap= 0.138 Goal= None Shift= 0.000

Gap= 0.231 Goal= None Shift= 0.000

RMSDP=1.12D-03 MaxDP=5.89D-02 DE=-1.61D-01 OVMax= 1.47D-01

Cycle 3 Pass 1 IDiag 1:

RMSU= 9.81D-04 CP: 9.84D-01 7.61D-01

E= -1658.64772783439 Delta-E= -0.261972504619 Rises=F Damp=F

DIIS: error= 1.31D-02 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.64772783439 IErMin= 2 ErrMin= 8.62D-03

ErrMax= 1.31D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.47D-01 BMatP= 1.98D-01

IDIUse=3 WtCom= 8.69D-01 WtEn= 1.31D-01

Coeff-Com: 0.228D-01 0.457D+00 0.520D+00

Coeff-En: 0.000D+00 0.000D+00 0.100D+01

Coeff: 0.198D-01 0.398D+00 0.583D+00

Gap= 0.107 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=7.18D-04 MaxDP=3.52D-02 DE=-2.62D-01 OVMax= 9.29D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 5.03D-04 CP: 9.86D-01 8.43D-01 5.13D-01

E= -1658.66232942375 Delta-E= -0.014601589362 Rises=F Damp=F

DIIS: error= 1.02D-02 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.66232942375 IErMin= 2 ErrMin= 8.62D-03

ErrMax= 1.02D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.31D-02 BMatP= 1.47D-01

IDIUse=3 WtCom= 8.98D-01 WtEn= 1.02D-01

Coeff-Com: -0.132D-01 0.931D-01 0.418D+00 0.502D+00

Coeff-En: 0.000D+00 0.000D+00 0.364D+00 0.636D+00

Coeff: -0.118D-01 0.836D-01 0.413D+00 0.516D+00

Gap= 0.114 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=3.75D-04 MaxDP=2.25D-02 DE=-1.46D-02 OVMax= 4.15D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.92D-04 CP: 9.84D-01 8.18D-01 7.31D-01 5.35D-01

E= -1658.67625961304 Delta-E= -0.013930189282 Rises=F Damp=F

DIIS: error= 1.40D-03 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67625961304 IErMin= 5 ErrMin= 1.40D-03

ErrMax= 1.40D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.96D-03 BMatP= 7.31D-02

IDIUse=3 WtCom= 9.86D-01 WtEn= 1.40D-02

Coeff-Com: -0.531D-02 0.192D-01 0.174D+00 0.264D+00 0.548D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.523D-02 0.190D-01 0.172D+00 0.260D+00 0.554D+00

Gap= 0.117 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=7.71D-05 MaxDP=3.31D-03 DE=-1.39D-02 OVMax= 8.21D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 5.72D-05 CP: 9.84D-01 8.17D-01 7.59D-01 6.04D-01 8.64D-01

E= -1658.67666492079 Delta-E= -0.000405307748 Rises=F Damp=F

DIIS: error= 3.27D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67666492079 IErMin= 6 ErrMin= 3.27D-04

ErrMax= 3.27D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.69D-04 BMatP= 1.96D-03

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.27D-03

Coeff-Com: -0.723D-03-0.300D-02 0.289D-01 0.587D-01 0.260D+00 0.656D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.721D-03-0.299D-02 0.288D-01 0.585D-01 0.259D+00 0.657D+00

Gap= 0.116 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=2.87D-05 MaxDP=1.22D-03 DE=-4.05D-04 OVMax= 3.46D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.22D-05 CP: 9.84D-01 8.16D-01 7.69D-01 6.24D-01 9.18D-01

CP: 1.03D+00

E= -1658.67671086805 Delta-E= -0.000045947263 Rises=F Damp=F

DIIS: error= 9.79D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67671086805 IErMin= 7 ErrMin= 9.79D-05

ErrMax= 9.79D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.86D-05 BMatP= 1.69D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.283D-03-0.392D-02-0.352D-02 0.154D-02 0.668D-01 0.305D+00

Coeff-Com: 0.634D+00

Coeff: 0.283D-03-0.392D-02-0.352D-02 0.154D-02 0.668D-01 0.305D+00

Coeff: 0.634D+00

Gap= 0.117 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=2.36D-05 MaxDP=1.03D-03 DE=-4.59D-05 OVMax= 3.83D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.13D-05 CP: 9.84D-01 8.14D-01 7.78D-01 6.25D-01 9.96D-01

CP: 1.23D+00 9.85D-01

E= -1658.67672156063 Delta-E= -0.000010692583 Rises=F Damp=F

DIIS: error= 8.69D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67672156063 IErMin= 8 ErrMin= 8.69D-05

ErrMax= 8.69D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.76D-06 BMatP= 2.86D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.507D-03-0.142D-02-0.125D-01-0.196D-01-0.481D-01-0.585D-01

Coeff-Com: 0.361D+00 0.778D+00

Coeff: 0.507D-03-0.142D-02-0.125D-01-0.196D-01-0.481D-01-0.585D-01

Coeff: 0.361D+00 0.778D+00

Gap= 0.117 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=1.29D-05 MaxDP=6.84D-04 DE=-1.07D-05 OVMax= 2.05D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 4.91D-06 CP: 9.84D-01 8.13D-01 7.82D-01 6.32D-01 1.03D+00

CP: 1.33D+00 1.24D+00 8.49D-01

E= -1658.67672598986 Delta-E= -0.000004429230 Rises=F Damp=F

DIIS: error= 3.43D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67672598986 IErMin= 9 ErrMin= 3.43D-05

ErrMax= 3.43D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.42D-06 BMatP= 9.76D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.314D-03-0.147D-03-0.829D-02-0.141D-01-0.470D-01-0.102D+00

Coeff-Com: 0.989D-01 0.512D+00 0.560D+00

Coeff: 0.314D-03-0.147D-03-0.829D-02-0.141D-01-0.470D-01-0.102D+00

Coeff: 0.989D-01 0.512D+00 0.560D+00

Gap= 0.117 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=6.83D-06 MaxDP=3.05D-04 DE=-4.43D-06 OVMax= 1.12D-03

Cycle 10 Pass 1 IDiag 1:

RMSU= 2.01D-06 CP: 9.84D-01 8.13D-01 7.85D-01 6.33D-01 1.04D+00

CP: 1.39D+00 1.35D+00 1.10D+00 8.19D-01

E= -1658.67672702657 Delta-E= -0.000001036710 Rises=F Damp=F

DIIS: error= 9.07D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67672702657 IErMin=10 ErrMin= 9.07D-06

ErrMax= 9.07D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.53D-07 BMatP= 3.42D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.498D-04 0.149D-03-0.184D-02-0.319D-02-0.140D-01-0.366D-01

Coeff-Com: -0.977D-02 0.135D+00 0.247D+00 0.683D+00

Coeff: 0.498D-04 0.149D-03-0.184D-02-0.319D-02-0.140D-01-0.366D-01

Coeff: -0.977D-02 0.135D+00 0.247D+00 0.683D+00

Gap= 0.117 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=1.37D-06 MaxDP=8.77D-05 DE=-1.04D-06 OVMax= 2.27D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 9.29D-07 CP: 9.84D-01 8.13D-01 7.86D-01 6.34D-01 1.04D+00

CP: 1.40D+00 1.36D+00 1.12D+00 9.46D-01 9.11D-01

E= -1658.67672710321 Delta-E= -0.000000076640 Rises=F Damp=F

DIIS: error= 5.95D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67672710321 IErMin=11 ErrMin= 5.95D-06

ErrMax= 5.95D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.72D-08 BMatP= 2.53D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.450D-04 0.115D-03 0.672D-03 0.110D-02 0.151D-02 0.997D-03

Coeff-Com: -0.249D-01-0.279D-01-0.504D-02 0.363D+00 0.691D+00

Coeff: -0.450D-04 0.115D-03 0.672D-03 0.110D-02 0.151D-02 0.997D-03

Coeff: -0.249D-01-0.279D-01-0.504D-02 0.363D+00 0.691D+00

Gap= 0.117 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=7.60D-07 MaxDP=3.77D-05 DE=-7.66D-08 OVMax= 8.19D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 3.55D-07 CP: 9.84D-01 8.13D-01 7.86D-01 6.34D-01 1.04D+00

CP: 1.40D+00 1.37D+00 1.15D+00 9.86D-01 1.11D+00

CP: 9.36D-01

E= -1658.67672712529 Delta-E= -0.000000022077 Rises=F Damp=F

DIIS: error= 1.70D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.67672712529 IErMin=12 ErrMin= 1.70D-06

ErrMax= 1.70D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.43D-09 BMatP= 6.72D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.169D-04 0.125D-04 0.463D-03 0.743D-03 0.247D-02 0.580D-02

Coeff-Com: -0.585D-02-0.263D-01-0.409D-01 0.289D-01 0.227D+00 0.807D+00

Coeff: -0.169D-04 0.125D-04 0.463D-03 0.743D-03 0.247D-02 0.580D-02

Coeff: -0.585D-02-0.263D-01-0.409D-01 0.289D-01 0.227D+00 0.807D+00

Gap= 0.117 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=2.55D-07 MaxDP=1.56D-05 DE=-2.21D-08 OVMax= 3.83D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.20D-07 CP: 9.84D-01 8.13D-01 7.86D-01 6.33D-01 1.04D+00

CP: 1.40D+00 1.37D+00 1.15D+00 1.00D+00 1.18D+00

CP: 1.09D+00 9.55D-01

E= -1658.67672712734 Delta-E= -0.000000002051 Rises=F Damp=F

DIIS: error= 5.04D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1658.67672712734 IErMin=13 ErrMin= 5.04D-07

ErrMax= 5.04D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.08D-10 BMatP= 4.43D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.304D-05-0.135D-04 0.334D-04 0.317D-04 0.443D-03 0.112D-02

Coeff-Com: 0.152D-02-0.195D-02-0.932D-02-0.396D-01-0.398D-01 0.228D+00

Coeff-Com: 0.859D+00

Coeff: 0.304D-05-0.135D-04 0.334D-04 0.317D-04 0.443D-03 0.112D-02

Coeff: 0.152D-02-0.195D-02-0.932D-02-0.396D-01-0.398D-01 0.228D+00

Coeff: 0.859D+00

Gap= 0.117 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=9.52D-08 MaxDP=5.46D-06 DE=-2.05D-09 OVMax= 1.75D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 3.92D-08 CP: 9.84D-01 8.13D-01 7.86D-01 6.33D-01 1.04D+00

CP: 1.40D+00 1.37D+00 1.15D+00 1.01D+00 1.20D+00

CP: 1.14D+00 1.10D+00 1.02D+00

E= -1658.67672712758 Delta-E= -0.000000000244 Rises=F Damp=F

DIIS: error= 2.42D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1658.67672712758 IErMin=14 ErrMin= 2.42D-07

ErrMax= 2.42D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.67D-11 BMatP= 5.08D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.304D-05-0.707D-05-0.308D-04-0.602D-04-0.402D-04-0.102D-03

Coeff-Com: 0.111D-02 0.189D-02-0.155D-03-0.207D-01-0.423D-01 0.248D-01

Coeff-Com: 0.395D+00 0.641D+00

Coeff: 0.304D-05-0.707D-05-0.308D-04-0.602D-04-0.402D-04-0.102D-03

Coeff: 0.111D-02 0.189D-02-0.155D-03-0.207D-01-0.423D-01 0.248D-01

Coeff: 0.395D+00 0.641D+00

Gap= 0.117 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=2.56D-08 MaxDP=1.46D-06 DE=-2.44D-10 OVMax= 2.56D-06

Cycle 15 Pass 1 IDiag 1:

RMSU= 1.42D-08 CP: 9.84D-01 8.13D-01 7.86D-01 6.33D-01 1.04D+00

CP: 1.40D+00 1.37D+00 1.15D+00 1.01D+00 1.20D+00

CP: 1.14D+00 1.13D+00 1.11D+00 9.19D-01

E= -1658.67672712762 Delta-E= -0.000000000040 Rises=F Damp=F

DIIS: error= 8.55D-08 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1658.67672712762 IErMin=15 ErrMin= 8.55D-08

ErrMax= 8.55D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.65D-12 BMatP= 9.67D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.344D-06-0.363D-06-0.130D-04-0.203D-04-0.629D-04-0.159D-03

Coeff-Com: 0.107D-03 0.863D-03 0.992D-03-0.105D-02-0.779D-02-0.219D-01

Coeff-Com: 0.127D-01 0.202D+00 0.815D+00

Coeff: 0.344D-06-0.363D-06-0.130D-04-0.203D-04-0.629D-04-0.159D-03

Coeff: 0.107D-03 0.863D-03 0.992D-03-0.105D-02-0.779D-02-0.219D-01

Coeff: 0.127D-01 0.202D+00 0.815D+00

Gap= 0.117 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=9.46D-09 MaxDP=5.83D-07 DE=-4.00D-11 OVMax= 1.51D-06

Error on total polarization charges = 0.04175

SCF Done: E(UB3LYP) = -1658.67672713 A.U. after 15 cycles

NFock= 15 Conv=0.95D-08 -V/T= 2.0022

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7553 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655117852552D+03 PE=-6.139001322099D+03 EE= 1.727040035599D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.58

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7553, after 0.7500

Leave Link 502 at Sat Aug 17 17:28:55 2019, MaxMem= 1342177280 cpu: 369.7

(Enter /apps/gaussian/g09d01/g09/l601.exe)

Copying SCF densities to generalized density rwf, IOpCl= 1 IROHF=0.

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Population analysis using the SCF density.

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Orbital symmetries:

Alpha Orbitals:

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Beta Orbitals:

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The electronic state is 2-A.

Alpha occ. eigenvalues -- -88.83330 -88.82928 -88.77125 -19.16171 -19.10170

Alpha occ. eigenvalues -- -10.29950 -10.20673 -10.19981 -10.17716 -10.15867

Alpha occ. eigenvalues -- -10.15623 -10.15491 -10.14775 -7.91870 -7.91501

Alpha occ. eigenvalues -- -7.85741 -5.88259 -5.87881 -5.87855 -5.87496

Alpha occ. eigenvalues -- -5.87277 -5.87005 -5.82090 -5.81740 -5.81325

Alpha occ. eigenvalues -- -1.10344 -1.00994 -0.82055 -0.80064 -0.77312

Alpha occ. eigenvalues -- -0.73290 -0.68091 -0.66403 -0.65368 -0.60720

Alpha occ. eigenvalues -- -0.58705 -0.57154 -0.49742 -0.48288 -0.47339

Alpha occ. eigenvalues -- -0.46917 -0.44921 -0.42634 -0.42020 -0.41698

Alpha occ. eigenvalues -- -0.40820 -0.39620 -0.38346 -0.37731 -0.36568

Alpha occ. eigenvalues -- -0.35979 -0.35448 -0.33836 -0.32849 -0.32414

Alpha occ. eigenvalues -- -0.32110 -0.31904 -0.29553 -0.28030 -0.26946

Alpha occ. eigenvalues -- -0.22918 -0.21269 -0.18774 -0.12700

Alpha virt. eigenvalues -- -0.01000 0.02665 0.04134 0.05190 0.06060

Alpha virt. eigenvalues -- 0.06935 0.07696 0.08518 0.08705 0.09349

Alpha virt. eigenvalues -- 0.10299 0.10514 0.11132 0.12403 0.13137

Alpha virt. eigenvalues -- 0.14228 0.14645 0.14928 0.15181 0.16844

Alpha virt. eigenvalues -- 0.17684 0.18286 0.20139 0.21010 0.22328

Alpha virt. eigenvalues -- 0.22887 0.23770 0.24324 0.24531 0.25258

Alpha virt. eigenvalues -- 0.26577 0.27067 0.28764 0.30003 0.30584

Alpha virt. eigenvalues -- 0.31369 0.31848 0.33707 0.34222 0.35038

Alpha virt. eigenvalues -- 0.36211 0.36574 0.37536 0.38386 0.41091

Alpha virt. eigenvalues -- 0.41873 0.44307 0.45468 0.47681 0.48512

Alpha virt. eigenvalues -- 0.49515 0.51756 0.51943 0.53375 0.53843

Alpha virt. eigenvalues -- 0.55630 0.56667 0.57227 0.58905 0.59394

Alpha virt. eigenvalues -- 0.59560 0.59842 0.60155 0.61188 0.61406

Alpha virt. eigenvalues -- 0.61803 0.62112 0.62761 0.62855 0.63372

Alpha virt. eigenvalues -- 0.63987 0.64164 0.65973 0.66893 0.67575

Alpha virt. eigenvalues -- 0.69420 0.69905 0.72771 0.75541 0.77077

Alpha virt. eigenvalues -- 0.79627 0.79868 0.80722 0.80942 0.83485

Alpha virt. eigenvalues -- 0.84447 0.86156 0.88254 0.90099 0.91240

Alpha virt. eigenvalues -- 0.91670 0.93035 0.94071 0.94702 0.95968

Alpha virt. eigenvalues -- 0.97467 0.97907 0.99170 1.01099 1.01998

Alpha virt. eigenvalues -- 1.04937 1.06163 1.08918 1.11163 1.13602

Alpha virt. eigenvalues -- 1.14122 1.18305 1.18714 1.20275 1.24745

Alpha virt. eigenvalues -- 1.32041 1.35437 1.39539 1.43824 1.46951

Alpha virt. eigenvalues -- 1.47153 1.47477 1.48771 1.51266 1.52199

Alpha virt. eigenvalues -- 1.52919 1.53918 1.54630 1.55652 1.58375

Alpha virt. eigenvalues -- 1.58990 1.62207 1.63054 1.63885 1.64619

Alpha virt. eigenvalues -- 1.65662 1.66126 1.67259 1.67602 1.69627

Alpha virt. eigenvalues -- 1.70643 1.72371 1.74988 1.77442 1.79453

Alpha virt. eigenvalues -- 1.81242 1.81767 1.83936 1.86798 1.86915

Alpha virt. eigenvalues -- 1.89219 1.90987 1.91970 1.94859 1.95516

Alpha virt. eigenvalues -- 1.97472 1.98206 2.00864 2.05720 2.11936

Alpha virt. eigenvalues -- 2.15288 2.17573 2.20611 2.37756 2.39476

Alpha virt. eigenvalues -- 2.39660 2.41558 2.41916 2.43439 2.43603

Alpha virt. eigenvalues -- 2.47016 2.49777 2.50635 2.51923 2.52758

Alpha virt. eigenvalues -- 2.54549 2.59086 2.73591 2.77170 2.84723

Alpha virt. eigenvalues -- 2.85030 2.87734 2.90941 2.92338 2.94061

Alpha virt. eigenvalues -- 2.97990 3.00075 3.02974 3.06659 3.08764

Alpha virt. eigenvalues -- 3.10560 3.11200 3.12937 3.14833 3.15176

Alpha virt. eigenvalues -- 3.18218 3.19936 3.20326 3.22573 3.25787

Alpha virt. eigenvalues -- 3.32322 3.33772 3.50364 3.55009 3.62123

Alpha virt. eigenvalues -- 3.72042 3.85542 3.88608 4.04738 4.06313

Alpha virt. eigenvalues -- 4.80274 4.90841 4.96259 5.06877 5.36170

Alpha virt. eigenvalues -- 5.66849 7.69537 7.82369 7.85603 17.27980

Alpha virt. eigenvalues -- 17.30116 17.30542 17.33258 17.36890 17.41420

Alpha virt. eigenvalues -- 17.44204 17.45750 17.49800 23.36789 23.40128

Alpha virt. eigenvalues -- 23.46640 23.56340 23.66993 23.68945 23.72735

Alpha virt. eigenvalues -- 23.77104 49.81632 49.97909 188.82102 188.95632

Alpha virt. eigenvalues -- 189.00115

Beta occ. eigenvalues -- -88.83329 -88.82880 -88.76997 -19.16159 -19.10139

Beta occ. eigenvalues -- -10.29930 -10.19821 -10.19753 -10.17695 -10.15867

Beta occ. eigenvalues -- -10.15623 -10.15496 -10.14775 -7.91864 -7.91458

Beta occ. eigenvalues -- -7.85626 -5.88284 -5.87906 -5.87835 -5.87477

Beta occ. eigenvalues -- -5.87232 -5.86842 -5.82043 -5.81318 -5.81252

Beta occ. eigenvalues -- -1.10306 -1.00945 -0.81447 -0.79945 -0.76796

Beta occ. eigenvalues -- -0.72928 -0.67949 -0.66210 -0.64943 -0.60521

Beta occ. eigenvalues -- -0.58587 -0.57125 -0.48797 -0.48135 -0.47242

Beta occ. eigenvalues -- -0.46886 -0.44545 -0.42515 -0.41889 -0.41618

Beta occ. eigenvalues -- -0.40672 -0.39350 -0.38204 -0.37482 -0.36418

Beta occ. eigenvalues -- -0.35628 -0.35261 -0.33429 -0.32441 -0.32104

Beta occ. eigenvalues -- -0.32071 -0.31430 -0.29163 -0.27588 -0.25375

Beta occ. eigenvalues -- -0.22567 -0.19808 -0.18439

Beta virt. eigenvalues -- -0.04894 0.00060 0.03322 0.04453 0.05375

Beta virt. eigenvalues -- 0.06259 0.07269 0.07759 0.08582 0.08961

Beta virt. eigenvalues -- 0.09595 0.10530 0.10680 0.11209 0.12443

Beta virt. eigenvalues -- 0.13221 0.14292 0.14677 0.14983 0.15214

Beta virt. eigenvalues -- 0.16911 0.17848 0.18525 0.20313 0.21169

Beta virt. eigenvalues -- 0.22529 0.23062 0.23880 0.24573 0.24704

Beta virt. eigenvalues -- 0.25460 0.26731 0.27418 0.29054 0.30206

Beta virt. eigenvalues -- 0.30696 0.31425 0.32137 0.33985 0.34252

Beta virt. eigenvalues -- 0.35126 0.36327 0.36650 0.37609 0.38526

Beta virt. eigenvalues -- 0.41189 0.42051 0.44524 0.45599 0.47838

Beta virt. eigenvalues -- 0.49267 0.49707 0.51976 0.52468 0.53471

Beta virt. eigenvalues -- 0.54174 0.55758 0.56859 0.57648 0.59024

Beta virt. eigenvalues -- 0.59417 0.59633 0.59873 0.60224 0.61376

Beta virt. eigenvalues -- 0.61620 0.61898 0.62262 0.62824 0.62902

Beta virt. eigenvalues -- 0.63451 0.64059 0.64274 0.66160 0.67171

Beta virt. eigenvalues -- 0.67800 0.69842 0.70431 0.73160 0.75634

Beta virt. eigenvalues -- 0.77644 0.79832 0.80035 0.80982 0.81542

Beta virt. eigenvalues -- 0.83690 0.85004 0.87078 0.88791 0.90405

Beta virt. eigenvalues -- 0.91448 0.92269 0.93261 0.94365 0.94910

Beta virt. eigenvalues -- 0.96244 0.97653 0.98345 0.99464 1.01207

Beta virt. eigenvalues -- 1.02819 1.05212 1.06332 1.09164 1.11388

Beta virt. eigenvalues -- 1.13781 1.14407 1.18385 1.18820 1.20475

Beta virt. eigenvalues -- 1.24880 1.32103 1.35517 1.39562 1.44369

Beta virt. eigenvalues -- 1.47084 1.48003 1.48173 1.48995 1.51798

Beta virt. eigenvalues -- 1.52645 1.52972 1.54349 1.55113 1.55975

Beta virt. eigenvalues -- 1.58442 1.59139 1.62378 1.63207 1.64132

Beta virt. eigenvalues -- 1.64912 1.66054 1.66336 1.67584 1.68076

Beta virt. eigenvalues -- 1.70047 1.71124 1.73338 1.75395 1.77826

Beta virt. eigenvalues -- 1.79518 1.81259 1.82126 1.84315 1.87011

Beta virt. eigenvalues -- 1.87262 1.89529 1.91195 1.92307 1.95202

Beta virt. eigenvalues -- 1.96204 1.97726 1.98498 2.01146 2.06277

Beta virt. eigenvalues -- 2.11992 2.15383 2.17899 2.20683 2.37760

Beta virt. eigenvalues -- 2.39488 2.39668 2.41594 2.41939 2.43513

Beta virt. eigenvalues -- 2.43654 2.47113 2.49925 2.50645 2.51965

Beta virt. eigenvalues -- 2.52769 2.54564 2.59211 2.75267 2.78990

Beta virt. eigenvalues -- 2.84799 2.85544 2.87823 2.90977 2.92402

Beta virt. eigenvalues -- 2.94122 2.98120 3.00489 3.03370 3.06786

Beta virt. eigenvalues -- 3.08769 3.10802 3.11261 3.13507 3.15102

Beta virt. eigenvalues -- 3.15234 3.18259 3.19974 3.20363 3.22648

Beta virt. eigenvalues -- 3.25808 3.32399 3.33822 3.50414 3.55049

Beta virt. eigenvalues -- 3.62131 3.72136 3.85554 3.88628 4.04744

Beta virt. eigenvalues -- 4.06438 4.80327 4.90955 4.96290 5.06890

Beta virt. eigenvalues -- 5.36204 5.66874 7.69682 7.82539 7.85683

Beta virt. eigenvalues -- 17.28162 17.30519 17.30719 17.33379 17.36892

Beta virt. eigenvalues -- 17.41416 17.44248 17.45768 17.49860 23.36877

Beta virt. eigenvalues -- 23.41030 23.46727 23.56350 23.66999 23.69032

Beta virt. eigenvalues -- 23.72737 23.77175 49.81646 49.97937 188.82172

Beta virt. eigenvalues -- 188.95709 189.00136

Condensed to atoms (all electrons):

1 2 3 4 5 6

1 C 4.515303 0.281325 0.643009 0.302946 -0.035823 -0.045358

2 C 0.281325 5.788393 -0.090752 -0.100739 0.206935 0.149406

3 O 0.643009 -0.090752 7.878956 -0.089173 0.003776 0.007115

4 O 0.302946 -0.100739 -0.089173 8.121572 0.006227 0.008129

5 C -0.035823 0.206935 0.003776 0.006227 5.404735 -0.072173

6 S -0.045358 0.149406 0.007115 0.008129 -0.072173 15.949384

7 C 0.004082 -0.055607 -0.000075 -0.000009 -0.005928 0.266114

8 S -0.000032 -0.015230 0.000022 -0.000060 0.005831 -0.131917

9 S 0.000141 -0.014611 -0.000126 -0.000058 -0.002794 -0.140452

10 C 0.000000 -0.000067 0.000000 0.000000 -0.000021 -0.000072

11 C 0.000000 0.000000 0.000000 0.000000 0.000001 -0.000212

12 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000017

13 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

14 H -0.053755 0.383473 0.009375 0.004755 -0.048695 -0.064988

15 H -0.035423 0.015494 0.012942 0.244808 -0.001476 -0.000862

16 H 0.006566 -0.038338 -0.000205 0.000080 0.391298 -0.014735

17 H -0.004371 -0.034151 0.000192 0.001227 0.374015 0.010619

18 H -0.007159 -0.036956 0.000202 0.007890 0.386258 -0.005355

19 H 0.000000 0.000025 0.000000 0.000000 -0.000002 0.004674

20 H 0.000000 -0.000015 0.000000 0.000000 0.000005 -0.001556

21 H 0.000000 0.000000 0.000000 0.000000 -0.000001 0.000007

22 H 0.000000 -0.000001 0.000000 0.000000 0.000000 -0.000223

23 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000007

24 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000001

25 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

26 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

27 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

7 8 9 10 11 12

1 C 0.004082 -0.000032 0.000141 0.000000 0.000000 0.000000

2 C -0.055607 -0.015230 -0.014611 -0.000067 0.000000 0.000000

3 O -0.000075 0.000022 -0.000126 0.000000 0.000000 0.000000

4 O -0.000009 -0.000060 -0.000058 0.000000 0.000000 0.000000

5 C -0.005928 0.005831 -0.002794 -0.000021 0.000001 0.000000

6 S 0.266114 -0.131917 -0.140452 -0.000072 -0.000212 0.000017

7 C 6.041520 0.142879 0.213310 -0.046717 0.004110 -0.000206

8 S 0.142879 15.963160 -0.116032 0.209463 -0.057504 0.008610

9 S 0.213310 -0.116032 16.555505 -0.019743 0.002341 0.000316

10 C -0.046717 0.209463 -0.019743 5.517101 0.308829 -0.060972

11 C 0.004110 -0.057504 0.002341 0.308829 5.275732 0.323104

12 C -0.000206 0.008610 0.000316 -0.060972 0.323104 5.216343

13 C 0.000002 -0.000527 0.000004 0.006865 -0.070373 0.328340

14 H -0.014865 -0.000034 0.022293 0.000012 0.000000 0.000000

15 H 0.000039 0.000000 0.000009 0.000000 0.000000 0.000000

16 H 0.003428 -0.000591 0.001458 -0.000188 -0.000002 0.000000

17 H -0.000304 0.000085 -0.000282 0.000000 0.000000 0.000000

18 H -0.001268 0.000420 0.000442 -0.000008 0.000000 0.000000

19 H 0.005046 -0.065142 -0.003784 0.356559 -0.031050 -0.007788

20 H -0.008429 -0.067119 0.005970 0.374237 -0.035797 -0.005797

21 H -0.000063 0.001242 -0.000182 -0.043774 0.395477 -0.044224

22 H -0.000324 -0.001330 -0.000279 -0.041892 0.395791 -0.044608

23 H -0.000018 -0.000282 0.000082 -0.004722 -0.045841 0.399538

24 H 0.000012 -0.000105 -0.000074 -0.004390 -0.044642 0.397813

25 H 0.000000 0.000035 0.000000 -0.000328 0.008085 -0.037572

26 H 0.000000 -0.000034 0.000001 -0.000140 -0.005547 -0.038956

27 H 0.000000 -0.000011 -0.000001 -0.000146 -0.005647 -0.039302

13 14 15 16 17 18

1 C 0.000000 -0.053755 -0.035423 0.006566 -0.004371 -0.007159

2 C 0.000000 0.383473 0.015494 -0.038338 -0.034151 -0.036956

3 O 0.000000 0.009375 0.012942 -0.000205 0.000192 0.000202

4 O 0.000000 0.004755 0.244808 0.000080 0.001227 0.007890

5 C 0.000000 -0.048695 -0.001476 0.391298 0.374015 0.386258

6 S 0.000000 -0.064988 -0.000862 -0.014735 0.010619 -0.005355

7 C 0.000002 -0.014865 0.000039 0.003428 -0.000304 -0.001268

8 S -0.000527 -0.000034 0.000000 -0.000591 0.000085 0.000420

9 S 0.000004 0.022293 0.000009 0.001458 -0.000282 0.000442

10 C 0.006865 0.000012 0.000000 -0.000188 0.000000 -0.000008

11 C -0.070373 0.000000 0.000000 -0.000002 0.000000 0.000000

12 C 0.328340 0.000000 0.000000 0.000000 0.000000 0.000000

13 C 5.298875 0.000000 0.000000 0.000000 0.000000 0.000000

14 H 0.000000 0.490886 -0.000774 -0.007766 -0.000896 0.006222

15 H 0.000000 -0.000774 0.350295 0.000103 -0.000280 -0.000229

16 H 0.000000 -0.007766 0.000103 0.473901 -0.032191 -0.024659

17 H 0.000000 -0.000896 -0.000280 -0.032191 0.491910 -0.029733

18 H 0.000000 0.006222 -0.000229 -0.024659 -0.029733 0.478463

19 H 0.000017 0.000021 0.000000 -0.000015 0.000001 0.000002

20 H -0.000067 -0.000023 0.000000 0.000145 -0.000003 -0.000002

21 H -0.003107 0.000000 0.000000 -0.000004 0.000000 0.000000

22 H -0.003508 0.000000 0.000000 0.000004 0.000000 0.000000

23 H -0.041401 0.000000 0.000000 0.000000 0.000000 0.000000

24 H -0.040792 0.000000 0.000000 0.000000 0.000000 0.000000

25 H 0.391681 0.000000 0.000000 0.000000 0.000000 0.000000

26 H 0.386685 0.000000 0.000000 0.000000 0.000000 0.000000

27 H 0.386952 0.000000 0.000000 0.000000 0.000000 0.000000

19 20 21 22 23 24

1 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

2 C 0.000025 -0.000015 0.000000 -0.000001 0.000000 0.000000

3 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

4 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

5 C -0.000002 0.000005 -0.000001 0.000000 0.000000 0.000000

6 S 0.004674 -0.001556 0.000007 -0.000223 -0.000007 0.000001

7 C 0.005046 -0.008429 -0.000063 -0.000324 -0.000018 0.000012

8 S -0.065142 -0.067119 0.001242 -0.001330 -0.000282 -0.000105

9 S -0.003784 0.005970 -0.000182 -0.000279 0.000082 -0.000074

10 C 0.356559 0.374237 -0.043774 -0.041892 -0.004722 -0.004390

11 C -0.031050 -0.035797 0.395477 0.395791 -0.045841 -0.044642

12 C -0.007788 -0.005797 -0.044224 -0.044608 0.399538 0.397813

13 C 0.000017 -0.000067 -0.003107 -0.003508 -0.041401 -0.040792

14 H 0.000021 -0.000023 0.000000 0.000000 0.000000 0.000000

15 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

16 H -0.000015 0.000145 -0.000004 0.000004 0.000000 0.000000

17 H 0.000001 -0.000003 0.000000 0.000000 0.000000 0.000000

18 H 0.000002 -0.000002 0.000000 0.000000 0.000000 0.000000

19 H 0.548971 -0.050256 0.008687 -0.006815 0.003419 -0.000265

20 H -0.050256 0.530520 -0.006448 0.008332 -0.000410 0.004143

21 H 0.008687 -0.006448 0.512539 -0.037524 0.008269 -0.007233

22 H -0.006815 0.008332 -0.037524 0.514605 -0.007049 0.008307

23 H 0.003419 -0.000410 0.008269 -0.007049 0.523138 -0.039416

24 H -0.000265 0.004143 -0.007233 0.008307 -0.039416 0.522014

25 H -0.000016 -0.000001 -0.000210 -0.000174 -0.004753 -0.004628

26 H -0.000015 0.000036 0.004373 -0.000420 0.008087 -0.006561

27 H 0.000061 -0.000009 -0.000386 0.004481 -0.006428 0.008044

25 26 27

1 C 0.000000 0.000000 0.000000

2 C 0.000000 0.000000 0.000000

3 O 0.000000 0.000000 0.000000

4 O 0.000000 0.000000 0.000000

5 C 0.000000 0.000000 0.000000

6 S 0.000000 0.000000 0.000000

7 C 0.000000 0.000000 0.000000

8 S 0.000035 -0.000034 -0.000011

9 S 0.000000 0.000001 -0.000001

10 C -0.000328 -0.000140 -0.000146

11 C 0.008085 -0.005547 -0.005647

12 C -0.037572 -0.038956 -0.039302

13 C 0.391681 0.386685 0.386952

14 H 0.000000 0.000000 0.000000

15 H 0.000000 0.000000 0.000000

16 H 0.000000 0.000000 0.000000

17 H 0.000000 0.000000 0.000000

18 H 0.000000 0.000000 0.000000

19 H -0.000016 -0.000015 0.000061

20 H -0.000001 0.000036 -0.000009

21 H -0.000210 0.004373 -0.000386

22 H -0.000174 -0.000420 0.004481

23 H -0.004753 0.008087 -0.006428

24 H -0.004628 -0.006561 0.008044

25 H 0.492831 -0.029929 -0.029903

26 H -0.029929 0.504375 -0.033080

27 H -0.029903 -0.033080 0.504185

Atomic-Atomic Spin Densities.

1 2 3 4 5 6

1 C 0.017699 0.001531 -0.005225 -0.002550 0.002450 0.001473

2 C 0.001531 0.214680 -0.001538 -0.001327 -0.023217 -0.094967

3 O -0.005225 -0.001538 0.015128 0.000393 -0.000067 0.001149

4 O -0.002550 -0.001327 0.000393 0.005842 -0.000105 0.000584

5 C 0.002450 -0.023217 -0.000067 -0.000105 0.004507 0.008282

6 S 0.001473 -0.094967 0.001149 0.000584 0.008282 0.114014

7 C 0.000674 -0.028673 -0.000008 0.000008 0.006208 0.027944

8 S 0.000071 -0.008242 0.000004 0.000021 0.001285 -0.014843

9 S -0.000835 0.009344 0.000058 0.000005 -0.000644 -0.010360

10 C 0.000000 -0.000077 0.000000 0.000000 0.000016 -0.004367

11 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000004

12 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000020

13 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

14 H -0.003208 0.009773 0.000669 0.000094 -0.001998 -0.013765

15 H 0.000084 -0.000496 0.000026 -0.000114 0.000103 0.000512

16 H 0.000213 -0.002170 -0.000007 -0.000008 0.001150 0.001266

17 H -0.001230 -0.000038 0.000067 0.000174 0.000672 -0.001415

18 H -0.000077 0.000639 0.000002 0.000014 -0.000147 0.000170

19 H 0.000000 0.000066 0.000000 0.000000 -0.000008 0.002934

20 H 0.000000 -0.000034 0.000000 0.000000 0.000007 -0.000800

21 H 0.000000 0.000001 0.000000 0.000000 0.000000 0.000046

22 H 0.000000 -0.000001 0.000000 0.000000 0.000000 -0.000083

23 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000007

24 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000002

25 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

26 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

27 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

7 8 9 10 11 12

1 C 0.000674 0.000071 -0.000835 0.000000 0.000000 0.000000

2 C -0.028673 -0.008242 0.009344 -0.000077 0.000000 0.000000

3 O -0.000008 0.000004 0.000058 0.000000 0.000000 0.000000

4 O 0.000008 0.000021 0.000005 0.000000 0.000000 0.000000

5 C 0.006208 0.001285 -0.000644 0.000016 0.000000 0.000000

6 S 0.027944 -0.014843 -0.010360 -0.004367 -0.000004 -0.000020

7 C 0.818822 -0.090719 -0.191683 -0.014120 0.000193 -0.000042

8 S -0.090719 0.190607 0.023333 -0.006853 -0.002528 -0.001157

9 S -0.191683 0.023333 0.421343 0.006487 -0.000293 0.000106

10 C -0.014120 -0.006853 0.006487 0.037548 -0.000331 0.000872

11 C 0.000193 -0.002528 -0.000293 -0.000331 0.000539 -0.000736

12 C -0.000042 -0.001157 0.000106 0.000872 -0.000736 0.001696

13 C 0.000000 0.000079 -0.000002 0.000006 0.000065 -0.000320

14 H -0.006319 -0.000680 0.008386 -0.000020 0.000000 0.000000

15 H 0.000007 0.000009 -0.000008 0.000000 0.000000 0.000000

16 H 0.003579 -0.000658 -0.003544 0.000062 0.000003 0.000000

17 H -0.000609 -0.000037 0.000765 -0.000001 0.000000 0.000000

18 H -0.000327 -0.000010 0.000132 -0.000003 0.000000 0.000000

19 H 0.014801 -0.001593 -0.012340 -0.019611 0.003185 -0.002190

20 H -0.001685 -0.009121 0.002483 0.007776 -0.000299 0.001162

21 H 0.000022 0.002062 -0.000012 -0.000922 -0.000190 -0.000541

22 H -0.000113 -0.000287 0.000069 0.000795 -0.000089 0.000483

23 H -0.000023 -0.000100 0.000069 0.000138 -0.000453 0.000677

24 H 0.000004 0.000145 -0.000018 0.000003 0.000061 -0.000312

25 H 0.000000 -0.000005 0.000000 0.000000 -0.000015 0.000034

26 H 0.000000 -0.000025 0.000000 0.000002 0.000003 0.000085

27 H 0.000000 0.000019 -0.000001 -0.000010 0.000064 -0.000116

13 14 15 16 17 18

1 C 0.000000 -0.003208 0.000084 0.000213 -0.001230 -0.000077

2 C 0.000000 0.009773 -0.000496 -0.002170 -0.000038 0.000639

3 O 0.000000 0.000669 0.000026 -0.000007 0.000067 0.000002

4 O 0.000000 0.000094 -0.000114 -0.000008 0.000174 0.000014

5 C 0.000000 -0.001998 0.000103 0.001150 0.000672 -0.000147

6 S 0.000000 -0.013765 0.000512 0.001266 -0.001415 0.000170

7 C 0.000000 -0.006319 0.000007 0.003579 -0.000609 -0.000327

8 S 0.000079 -0.000680 0.000009 -0.000658 -0.000037 -0.000010

9 S -0.000002 0.008386 -0.000008 -0.003544 0.000765 0.000132

10 C 0.000006 -0.000020 0.000000 0.000062 -0.000001 -0.000003

11 C 0.000065 0.000000 0.000000 0.000003 0.000000 0.000000

12 C -0.000320 0.000000 0.000000 0.000000 0.000000 0.000000

13 C 0.000382 0.000000 0.000000 0.000000 0.000000 0.000000

14 H 0.000000 0.004999 -0.000065 -0.000808 0.001099 0.000026

15 H 0.000000 -0.000065 -0.000049 0.000004 -0.000035 -0.000009

16 H 0.000000 -0.000808 0.000004 0.000611 -0.000646 -0.000180

17 H 0.000000 0.001099 -0.000035 -0.000646 0.003323 0.000241

18 H 0.000000 0.000026 -0.000009 -0.000180 0.000241 0.000014

19 H 0.000101 0.000017 0.000000 -0.000017 0.000000 0.000001

20 H -0.000061 -0.000016 0.000000 0.000027 -0.000001 -0.000001

21 H 0.000106 0.000000 0.000000 -0.000002 0.000000 0.000000

22 H -0.000072 0.000000 0.000000 0.000001 0.000000 0.000000

23 H -0.000151 0.000000 0.000000 0.000000 0.000000 0.000000

24 H 0.000105 0.000000 0.000000 0.000000 0.000000 0.000000

25 H -0.000031 0.000000 0.000000 0.000000 0.000000 0.000000

26 H -0.000074 0.000000 0.000000 0.000000 0.000000 0.000000

27 H 0.000043 0.000000 0.000000 0.000000 0.000000 0.000000

19 20 21 22 23 24

1 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

2 C 0.000066 -0.000034 0.000001 -0.000001 0.000000 0.000000

3 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

4 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

5 C -0.000008 0.000007 0.000000 0.000000 0.000000 0.000000

6 S 0.002934 -0.000800 0.000046 -0.000083 -0.000007 0.000002

7 C 0.014801 -0.001685 0.000022 -0.000113 -0.000023 0.000004

8 S -0.001593 -0.009121 0.002062 -0.000287 -0.000100 0.000145

9 S -0.012340 0.002483 -0.000012 0.000069 0.000069 -0.000018

10 C -0.019611 0.007776 -0.000922 0.000795 0.000138 0.000003

11 C 0.003185 -0.000299 -0.000190 -0.000089 -0.000453 0.000061

12 C -0.002190 0.001162 -0.000541 0.000483 0.000677 -0.000312

13 C 0.000101 -0.000061 0.000106 -0.000072 -0.000151 0.000105

14 H 0.000017 -0.000016 0.000000 0.000000 0.000000 0.000000

15 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

16 H -0.000017 0.000027 -0.000002 0.000001 0.000000 0.000000

17 H 0.000000 -0.000001 0.000000 0.000000 0.000000 0.000000

18 H 0.000001 -0.000001 0.000000 0.000000 0.000000 0.000000

19 H 0.028607 -0.006527 0.000437 -0.000717 -0.000750 0.000211

20 H -0.006527 0.006053 -0.000398 0.000197 0.000224 -0.000228

21 H 0.000437 -0.000398 -0.000029 -0.000111 -0.000066 0.000068

22 H -0.000717 0.000197 -0.000111 -0.000035 0.000087 -0.000030

23 H -0.000750 0.000224 -0.000066 0.000087 0.000396 -0.000108

24 H 0.000211 -0.000228 0.000068 -0.000030 -0.000108 0.000197

25 H -0.000009 0.000005 -0.000008 0.000008 0.000039 -0.000019

26 H -0.000010 0.000009 -0.000033 0.000014 0.000016 -0.000019

27 H 0.000031 -0.000009 0.000027 -0.000039 -0.000048 0.000014

25 26 27

1 C 0.000000 0.000000 0.000000

2 C 0.000000 0.000000 0.000000

3 O 0.000000 0.000000 0.000000

4 O 0.000000 0.000000 0.000000

5 C 0.000000 0.000000 0.000000

6 S 0.000000 0.000000 0.000000

7 C 0.000000 0.000000 0.000000

8 S -0.000005 -0.000025 0.000019

9 S 0.000000 0.000000 -0.000001

10 C 0.000000 0.000002 -0.000010

11 C -0.000015 0.000003 0.000064

12 C 0.000034 0.000085 -0.000116

13 C -0.000031 -0.000074 0.000043

14 H 0.000000 0.000000 0.000000

15 H 0.000000 0.000000 0.000000

16 H 0.000000 0.000000 0.000000

17 H 0.000000 0.000000 0.000000

18 H 0.000000 0.000000 0.000000

19 H -0.000009 -0.000010 0.000031

20 H 0.000005 0.000009 -0.000009

21 H -0.000008 -0.000033 0.000027

22 H 0.000008 0.000014 -0.000039

23 H 0.000039 0.000016 -0.000048

24 H -0.000019 -0.000019 0.000014

25 H 0.000004 0.000030 -0.000036

26 H 0.000030 0.000050 -0.000033

27 H -0.000036 -0.000033 0.000086

Mulliken charges and spin densities:

1 2

1 C 0.428549 0.011070

2 C -0.438582 0.075254

3 O -0.375256 0.010651

4 O -0.507595 0.003032

5 C -0.612166 -0.001503

6 S 0.082445 0.017745

7 C -0.546726 0.537942

8 S 0.124203 0.080778

9 S -0.503455 0.252836

10 C -0.549884 0.007390

11 C -0.416852 -0.000826

12 C -0.394656 -0.000321

13 C -0.639644 0.000177

14 H 0.274760 -0.001816

15 H 0.415353 -0.000031

16 H 0.241712 -0.001124

17 H 0.224162 0.002329

18 H 0.225471 0.000484

19 H 0.237664 0.006617

20 H 0.252544 -0.001237

21 H 0.212564 0.000454

22 H 0.212626 0.000076

23 H 0.207793 -0.000060

24 H 0.207771 0.000077

25 H 0.214883 -0.000002

26 H 0.211127 0.000016

27 H 0.211191 -0.000008

Sum of Mulliken charges = -1.00000 1.00000

Mulliken charges and spin densities with hydrogens summed into heavy atoms:

1 2

1 C 0.428549 0.011070

2 C -0.163823 0.073438

3 O -0.375256 0.010651

4 O -0.092242 0.003001

5 C 0.079179 0.000186

6 S 0.082445 0.017745

7 C -0.546726 0.537942

8 S 0.124203 0.080778

9 S -0.503455 0.252836

10 C -0.059675 0.012770

11 C 0.008338 -0.000296

12 C 0.020907 -0.000304

13 C -0.002443 0.000183

Electronic spatial extent (au): <R\*\*2>= 6098.0297

Charge= -1.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 3.5521 Y= -7.4658 Z= 1.1499 Tot= 8.3474

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -109.6983 YY= -128.4140 ZZ= -110.1119

XY= 12.8524 XZ= -6.1972 YZ= -0.1189

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= 6.3765 YY= -12.3393 ZZ= 5.9628

XY= 12.8524 XZ= -6.1972 YZ= -0.1189

Octapole moment (field-independent basis, Debye-Ang\*\*2):

XXX= -3.5997 YYY= -59.9917 ZZZ= -2.6825 XYY= -13.1846

XXY= -70.0987 XXZ= 9.7823 XZZ= -9.7706 YZZ= -11.4513

YYZ= -5.0621 XYZ= -13.3802

Hexadecapole moment (field-independent basis, Debye-Ang\*\*3):

XXXX= -6988.9832 YYYY= -1011.8149 ZZZZ= -430.0690 XXXY= 470.5247

XXXZ= -14.4148 YYYX= 45.4488 YYYZ= -0.9310 ZZZX= -1.9350

ZZZY= -6.4596 XXYY= -1311.7043 XXZZ= -1217.2998 YYZZ= -231.7271

XXYZ= 68.8781 YYXZ= 13.1225 ZZXY= 19.1662

N-N= 1.098166706820D+03 E-N=-6.139001311103D+03 KE= 1.655117852552D+03

Isotropic Fermi Contact Couplings

Atom a.u. MegaHertz Gauss 10(-4) cm-1

1 C(13) 0.00046 0.52074 0.18581 0.17370

2 C(13) 0.04397 49.42825 17.63723 16.48749

3 O(17) 0.00217 -1.31580 -0.46951 -0.43890

4 O(17) 0.00047 -0.28510 -0.10173 -0.09510

5 C(13) -0.00266 -2.98921 -1.06662 -0.99709

6 S(33) 0.08296 28.49368 10.16725 9.50447

7 C(13) 0.07664 86.15537 30.74238 28.73834

8 S(33) 0.00337 1.15645 0.41265 0.38575

9 S(33) 0.00771 2.64702 0.94452 0.88295

10 C(13) 0.00676 7.59422 2.70981 2.53316

11 C(13) -0.00104 -1.16356 -0.41519 -0.38812

12 C(13) 0.00017 0.19220 0.06858 0.06411

13 C(13) 0.00012 0.13933 0.04972 0.04647

14 H(1) -0.00091 -4.07145 -1.45279 -1.35809

15 H(1) -0.00011 -0.48083 -0.17157 -0.16039

16 H(1) 0.00018 0.78333 0.27951 0.26129

17 H(1) 0.00139 6.20986 2.21583 2.07139

18 H(1) 0.00039 1.75892 0.62763 0.58671

19 H(1) 0.00159 7.11767 2.53976 2.37420

20 H(1) 0.00032 1.41537 0.50504 0.47212

21 H(1) -0.00005 -0.21059 -0.07514 -0.07024

22 H(1) 0.00007 0.32433 0.11573 0.10818

23 H(1) 0.00011 0.48645 0.17358 0.16226

24 H(1) 0.00001 0.03290 0.01174 0.01097

25 H(1) -0.00001 -0.02546 -0.00908 -0.00849

26 H(1) 0.00000 -0.00790 -0.00282 -0.00263

27 H(1) 0.00000 -0.00758 -0.00270 -0.00253

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Center ---- Spin Dipole Couplings ----

3XX-RR 3YY-RR 3ZZ-RR

--------------------------------------------------------

1 Atom -0.008584 -0.012088 0.020672

2 Atom 0.018690 -0.049148 0.030459

3 Atom -0.026287 -0.022756 0.049043

4 Atom -0.002392 -0.007889 0.010281

5 Atom -0.000140 -0.001684 0.001824

6 Atom 0.026960 0.118934 -0.145893

7 Atom -0.223000 -0.303161 0.526161

8 Atom -0.214055 -0.260710 0.474765

9 Atom -0.123207 -0.500152 0.623359

10 Atom 0.015804 -0.004362 -0.011442

11 Atom 0.002027 -0.001956 -0.000071

12 Atom 0.001690 -0.000960 -0.000730

13 Atom 0.000950 -0.000369 -0.000581

14 Atom 0.002608 0.002061 -0.004669

15 Atom 0.001478 -0.000564 -0.000914

16 Atom -0.001388 -0.001923 0.003311

17 Atom 0.000222 -0.001262 0.001040

18 Atom -0.000359 0.001977 -0.001618

19 Atom 0.006504 -0.003447 -0.003057

20 Atom 0.004346 -0.001427 -0.002919

21 Atom 0.002660 -0.001195 -0.001464

22 Atom 0.001963 -0.000530 -0.001433

23 Atom 0.001627 -0.000827 -0.000801

24 Atom 0.001584 -0.000785 -0.000798

25 Atom 0.000659 -0.000311 -0.000348

26 Atom 0.000725 -0.000317 -0.000408

27 Atom 0.000694 -0.000282 -0.000413

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XY XZ YZ

--------------------------------------------------------

1 Atom 0.001272 0.000502 0.003081

2 Atom -0.008747 -0.074751 0.013251

3 Atom -0.003907 -0.002383 0.017076

4 Atom -0.002227 -0.010685 0.009198

5 Atom 0.002122 -0.002226 -0.002916

6 Atom -0.202283 0.039285 0.033878

7 Atom 0.095527 -0.356314 -0.234723

8 Atom 0.035400 0.188869 -0.027101

9 Atom 0.160344 -0.639729 -0.326479

10 Atom 0.009478 -0.004222 -0.002009

11 Atom -0.001053 0.001007 -0.001030

12 Atom -0.000432 0.000326 -0.000039

13 Atom -0.000466 -0.000008 -0.000003

14 Atom 0.000214 -0.004206 0.004829

15 Atom 0.001396 0.000861 0.000477

16 Atom 0.002183 -0.003507 -0.004634

17 Atom 0.000998 -0.001400 -0.001846

18 Atom 0.001676 -0.000847 -0.002531

19 Atom 0.000531 -0.002331 -0.001002

20 Atom 0.001439 0.002996 0.000861

21 Atom -0.001436 0.000655 -0.000584

22 Atom -0.001834 -0.000863 0.000343

23 Atom -0.000015 -0.000482 -0.000077

24 Atom 0.000083 0.000376 0.000002

25 Atom -0.000129 -0.000016 -0.000003

26 Atom -0.000363 0.000162 -0.000069

27 Atom -0.000404 -0.000156 0.000058

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Anisotropic Spin Dipole Couplings in Principal Axis System

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Atom a.u. MegaHertz Gauss 10(-4) cm-1 Axes

Baa -0.0127 -1.709 -0.610 -0.570 -0.2827 0.9555 -0.0839

1 C(13) Bbb -0.0082 -1.105 -0.394 -0.369 0.9590 0.2797 -0.0465

Bcc 0.0210 2.814 1.004 0.939 0.0209 0.0936 0.9954

Baa -0.0532 -7.133 -2.545 -2.379 -0.4493 0.7285 -0.5171

2 C(13) Bbb -0.0480 -6.445 -2.300 -2.150 0.5866 0.6772 0.4443

Bcc 0.1012 13.579 4.845 4.529 -0.6738 0.1037 0.7316

Baa -0.0298 2.156 0.769 0.719 0.6960 0.7058 -0.1318

3 O(17) Bbb -0.0232 1.681 0.600 0.561 0.7169 -0.6728 0.1826

Bcc 0.0530 -3.837 -1.369 -1.280 -0.0402 0.2216 0.9743

Baa -0.0125 0.902 0.322 0.301 -0.3343 0.8087 -0.4839

4 O(17) Bbb -0.0070 0.503 0.179 0.168 0.8319 0.4946 0.2518

Bcc 0.0194 -1.405 -0.501 -0.469 -0.4430 0.3184 0.8381

Baa -0.0036 -0.482 -0.172 -0.161 -0.3214 0.8826 0.3432

5 C(13) Bbb -0.0016 -0.212 -0.076 -0.071 0.8079 0.0665 0.5856

Bcc 0.0052 0.694 0.248 0.231 -0.4940 -0.4654 0.7344

Baa -0.1923 -7.886 -2.814 -2.631 -0.5196 -0.4187 0.7448

6 S(33) Bbb -0.0881 -3.610 -1.288 -1.204 0.5843 0.4618 0.6673

Bcc 0.2804 11.496 4.102 3.835 -0.6234 0.7819 0.0047

Baa -0.3669 -49.233 -17.568 -16.422 0.7308 -0.6729 0.1147

7 C(13) Bbb -0.3638 -48.817 -17.419 -16.283 0.5795 0.7004 0.4167

Bcc 0.7307 98.050 34.987 32.706 -0.3608 -0.2381 0.9018

Baa -0.3028 -12.414 -4.430 -4.141 -0.6869 0.7011 0.1913

8 S(33) Bbb -0.2208 -9.051 -3.230 -3.019 0.6835 0.7127 -0.1578

Bcc 0.5235 21.465 7.659 7.160 0.2470 -0.0223 0.9688

Baa -0.5892 -24.155 -8.619 -8.057 0.0880 0.9492 0.3020

9 S(33) Bbb -0.4853 -19.896 -7.099 -6.636 0.8716 -0.2202 0.4381

Bcc 1.0744 44.051 15.718 14.694 -0.4823 -0.2247 0.8467

Baa -0.0122 -1.631 -0.582 -0.544 0.1068 0.1244 0.9865

10 C(13) Bbb -0.0081 -1.086 -0.388 -0.362 -0.3791 0.9223 -0.0753

Bcc 0.0202 2.717 0.969 0.906 0.9192 0.3659 -0.1457

Baa -0.0025 -0.334 -0.119 -0.111 0.1417 0.9306 0.3374

11 C(13) Bbb -0.0003 -0.045 -0.016 -0.015 -0.4682 -0.2373 0.8512

Bcc 0.0028 0.379 0.135 0.127 0.8722 -0.2786 0.4020

Baa -0.0010 -0.138 -0.049 -0.046 0.1622 0.9856 -0.0480

12 C(13) Bbb -0.0008 -0.104 -0.037 -0.035 -0.1193 0.0679 0.9905

Bcc 0.0018 0.242 0.086 0.081 0.9795 -0.1550 0.1286

Baa -0.0006 -0.078 -0.028 -0.026 0.0270 0.0716 0.9971

13 C(13) Bbb -0.0005 -0.069 -0.025 -0.023 0.3017 0.9503 -0.0764

Bcc 0.0011 0.147 0.053 0.049 0.9530 -0.3029 -0.0040

Baa -0.0085 -4.553 -1.625 -1.519 0.3308 -0.3969 0.8562

14 H(1) Bbb 0.0026 1.373 0.490 0.458 0.7221 0.6906 0.0412

Bcc 0.0060 3.180 1.135 1.061 0.6076 -0.6046 -0.5151

Baa -0.0013 -0.686 -0.245 -0.229 -0.3320 0.8749 -0.3526

15 H(1) Bbb -0.0012 -0.633 -0.226 -0.211 -0.3981 0.2090 0.8932

Bcc 0.0025 1.319 0.471 0.440 0.8552 0.4369 0.2789

Baa -0.0046 -2.474 -0.883 -0.825 -0.0714 0.8751 0.4787

16 H(1) Bbb -0.0032 -1.720 -0.614 -0.574 0.9103 -0.1391 0.3899

Bcc 0.0079 4.194 1.496 1.399 -0.4078 -0.4636 0.7866

Baa -0.0023 -1.231 -0.439 -0.410 -0.1033 0.8886 0.4470

17 H(1) Bbb -0.0008 -0.416 -0.148 -0.139 0.8521 -0.1528 0.5006

Bcc 0.0031 1.646 0.587 0.549 -0.5131 -0.4326 0.7413

Baa -0.0029 -1.561 -0.557 -0.521 -0.0083 0.4611 0.8873

18 H(1) Bbb -0.0012 -0.615 -0.220 -0.205 0.9209 -0.3422 0.1865

Bcc 0.0041 2.176 0.776 0.726 0.3896 0.8187 -0.4217

Baa -0.0044 -2.349 -0.838 -0.784 0.1201 0.6856 0.7180

19 H(1) Bbb -0.0027 -1.436 -0.512 -0.479 -0.2084 0.7246 -0.6569

Bcc 0.0071 3.785 1.351 1.263 0.9706 0.0708 -0.2299

Baa -0.0040 -2.156 -0.769 -0.719 -0.3122 -0.1378 0.9400

20 H(1) Bbb -0.0018 -0.937 -0.335 -0.313 -0.2554 0.9652 0.0566

Bcc 0.0058 3.093 1.104 1.032 0.9151 0.2224 0.3365

Baa -0.0020 -1.057 -0.377 -0.353 0.1347 0.7374 0.6619

21 H(1) Bbb -0.0013 -0.689 -0.246 -0.230 -0.3369 -0.5941 0.7304

Bcc 0.0033 1.746 0.623 0.583 0.9318 -0.3214 0.1684

Baa -0.0017 -0.894 -0.319 -0.298 0.3812 0.3545 0.8539

22 H(1) Bbb -0.0014 -0.771 -0.275 -0.257 0.3177 0.8171 -0.4810

Bcc 0.0031 1.665 0.594 0.555 0.8682 -0.4547 -0.1988

Baa -0.0009 -0.504 -0.180 -0.168 0.1564 0.5535 0.8180

23 H(1) Bbb -0.0008 -0.413 -0.147 -0.138 -0.1038 0.8328 -0.5437

Bcc 0.0017 0.917 0.327 0.306 0.9822 -0.0001 -0.1877

Baa -0.0009 -0.458 -0.163 -0.153 -0.1554 0.1508 0.9763

24 H(1) Bbb -0.0008 -0.420 -0.150 -0.140 -0.0102 0.9880 -0.1542

Bcc 0.0016 0.877 0.313 0.293 0.9878 0.0339 0.1520

Baa -0.0003 -0.187 -0.067 -0.062 0.0467 0.2432 0.9688

25 H(1) Bbb -0.0003 -0.174 -0.062 -0.058 0.1220 0.9613 -0.2472

Bcc 0.0007 0.361 0.129 0.120 0.9914 -0.1297 -0.0153

Baa -0.0004 -0.239 -0.085 -0.080 0.1149 0.6904 0.7143

26 H(1) Bbb -0.0004 -0.221 -0.079 -0.074 -0.3069 -0.6592 0.6865

Bcc 0.0009 0.460 0.164 0.154 0.9448 -0.2981 0.1361

Baa -0.0004 -0.232 -0.083 -0.077 0.0700 -0.1837 0.9805

27 H(1) Bbb -0.0004 -0.228 -0.081 -0.076 0.3536 0.9236 0.1478

Bcc 0.0009 0.460 0.164 0.153 0.9328 -0.3364 -0.1296

---------------------------------------------------------------------------------

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Sat Aug 17 17:28:55 2019, MaxMem= 1342177280 cpu: 2.2

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 344

Leave Link 701 at Sat Aug 17 17:28:56 2019, MaxMem= 1342177280 cpu: 10.3

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:28:56 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:28:59 2019, MaxMem= 1342177280 cpu: 35.9

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.39750647D+00-2.93729031D+00 4.52400363D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.010953873 0.008150387 -0.006760785

2 6 -0.000095628 -0.000445442 0.001048395

3 8 0.010090494 -0.010470662 0.005759110

4 8 -0.000552108 0.002332889 -0.000483010

5 6 0.000143115 0.000713671 -0.000914771

6 16 0.000049048 0.000764283 0.001439646

7 6 -0.000686377 -0.000157905 0.000111608

8 16 0.000106574 0.000689251 0.000088225

9 16 -0.000036883 -0.000852232 -0.000365533

10 6 0.001166716 0.000945564 -0.000295342

11 6 -0.000119947 0.000018245 -0.000063728

12 6 -0.000037019 -0.000048482 -0.000006747

13 6 -0.000718891 0.000230322 -0.000026214

14 1 0.000025563 -0.001597400 -0.000765834

15 1 0.002715277 0.000980040 0.001293357

16 1 -0.001055419 -0.000723423 -0.000058984

17 1 0.001048048 -0.000386964 -0.000720361

18 1 -0.000243461 0.001317775 0.000526646

19 1 -0.000190419 -0.000707940 0.001488629

20 1 -0.000212465 -0.001235727 -0.001191532

21 1 -0.000040693 0.000358613 -0.001226157

22 1 -0.000021272 0.000691619 0.001090989

23 1 0.000053318 -0.000366549 0.001217072

24 1 0.000002552 -0.000651517 -0.001068084

25 1 -0.000998660 -0.000846984 0.000112733

26 1 0.000248730 0.000498431 -0.001259914

27 1 0.000313678 0.000800135 0.001030586

-------------------------------------------------------------------

Cartesian Forces: Max 0.010953873 RMS 0.002555895

Leave Link 716 at Sat Aug 17 17:28:59 2019, MaxMem= 1342177280 cpu: 0.3

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.015645556 RMS 0.001594303

Search for a local minimum.

Step number 1 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .15943D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Second derivative matrix not updated -- first step.

ITU= 0

Eigenvalues --- 0.00230 0.00230 0.00322 0.00367 0.00400

Eigenvalues --- 0.00442 0.00487 0.00754 0.00878 0.00943

Eigenvalues --- 0.01125 0.02306 0.03513 0.03595 0.04408

Eigenvalues --- 0.04817 0.04850 0.04898 0.05057 0.05473

Eigenvalues --- 0.05502 0.05565 0.05619 0.05829 0.08219

Eigenvalues --- 0.08328 0.08587 0.11225 0.12119 0.12201

Eigenvalues --- 0.13680 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.18503 0.19318

Eigenvalues --- 0.19818 0.21899 0.21904 0.22003 0.23320

Eigenvalues --- 0.24782 0.24992 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.26549 0.29096 0.29388 0.29408

Eigenvalues --- 0.29640 0.30261 0.32282 0.33275 0.33866

Eigenvalues --- 0.33874 0.33883 0.33907 0.34024 0.34032

Eigenvalues --- 0.34035 0.34122 0.34239 0.34455 0.34491

Eigenvalues --- 0.34522 0.34623 0.52295 0.54266 0.94802

RFO step: Lambda=-5.91001678D-04 EMin= 2.30000000D-03

Linear search not attempted -- first point.

Iteration 1 RMS(Cart)= 0.08186321 RMS(Int)= 0.00130044

Iteration 2 RMS(Cart)= 0.00338375 RMS(Int)= 0.00002464

Iteration 3 RMS(Cart)= 0.00000176 RMS(Int)= 0.00002462

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00002462

ITry= 1 IFail=0 DXMaxC= 2.55D-01 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83631 -0.00129 0.00000 -0.00398 -0.00398 2.83233

R2 2.30796 -0.01565 0.00000 -0.01649 -0.01649 2.29146

R3 2.55790 -0.00367 0.00000 -0.00676 -0.00676 2.55114

R4 2.87446 -0.00149 0.00000 -0.00491 -0.00491 2.86955

R5 3.60025 -0.00153 0.00000 -0.00788 -0.00788 3.59237

R6 2.06291 -0.00176 0.00000 -0.00507 -0.00507 2.05785

R7 1.84318 -0.00310 0.00000 -0.00593 -0.00593 1.83725

R8 2.06569 -0.00117 0.00000 -0.00338 -0.00338 2.06231

R9 2.07276 -0.00123 0.00000 -0.00362 -0.00362 2.06914

R10 2.06457 -0.00146 0.00000 -0.00422 -0.00422 2.06035

R11 3.32900 -0.00137 0.00000 -0.00465 -0.00465 3.32435

R12 3.39125 -0.00057 0.00000 -0.00216 -0.00216 3.38909

R13 3.25571 -0.00095 0.00000 -0.00284 -0.00284 3.25287

R14 3.47381 -0.00062 0.00000 -0.00264 -0.00264 3.47116

R15 2.88687 -0.00146 0.00000 -0.00492 -0.00492 2.88195

R16 2.06929 -0.00164 0.00000 -0.00477 -0.00477 2.06452

R17 2.06510 -0.00173 0.00000 -0.00502 -0.00502 2.06008

R18 2.89803 -0.00117 0.00000 -0.00402 -0.00402 2.89401

R19 2.07557 -0.00123 0.00000 -0.00362 -0.00362 2.07195

R20 2.07487 -0.00127 0.00000 -0.00375 -0.00375 2.07112

R21 2.89159 -0.00134 0.00000 -0.00453 -0.00453 2.88706

R22 2.07543 -0.00123 0.00000 -0.00362 -0.00362 2.07180

R23 2.07528 -0.00123 0.00000 -0.00361 -0.00361 2.07166

R24 2.07125 -0.00129 0.00000 -0.00378 -0.00378 2.06747

R25 2.07289 -0.00132 0.00000 -0.00387 -0.00387 2.06902

R26 2.07271 -0.00133 0.00000 -0.00389 -0.00389 2.06882

A1 2.17893 0.00051 0.00000 0.00209 0.00208 2.18101

A2 1.98016 -0.00173 0.00000 -0.00681 -0.00682 1.97334

A3 2.12359 0.00122 0.00000 0.00496 0.00495 2.12854

A4 2.01443 0.00037 0.00000 0.00144 0.00143 2.01586

A5 1.85565 -0.00045 0.00000 -0.00424 -0.00424 1.85141

A6 1.87066 -0.00002 0.00000 0.00165 0.00164 1.87230

A7 1.95021 -0.00003 0.00000 -0.00152 -0.00152 1.94869

A8 1.93975 0.00006 0.00000 0.00296 0.00295 1.94270

A9 1.82051 0.00003 0.00000 -0.00064 -0.00063 1.81987

A10 1.87731 -0.00117 0.00000 -0.00731 -0.00731 1.87000

A11 1.90922 0.00062 0.00000 0.00435 0.00435 1.91356

A12 1.92443 0.00050 0.00000 0.00297 0.00297 1.92739

A13 1.95071 -0.00012 0.00000 -0.00106 -0.00106 1.94965

A14 1.88514 -0.00048 0.00000 -0.00234 -0.00235 1.88279

A15 1.89534 -0.00024 0.00000 -0.00120 -0.00120 1.89415

A16 1.89761 -0.00031 0.00000 -0.00287 -0.00287 1.89474

A17 1.78485 0.00026 0.00000 0.00103 0.00103 1.78588

A18 1.96420 -0.00022 0.00000 0.00102 0.00086 1.96506

A19 2.14181 0.00013 0.00000 0.00247 0.00232 2.14412

A20 2.15816 0.00015 0.00000 0.00250 0.00234 2.16050

A21 1.79528 0.00010 0.00000 0.00038 0.00038 1.79567

A22 1.92489 -0.00032 0.00000 -0.00173 -0.00173 1.92316

A23 1.88209 -0.00003 0.00000 -0.00120 -0.00120 1.88089

A24 1.89327 0.00000 0.00000 -0.00080 -0.00080 1.89247

A25 1.93645 0.00022 0.00000 0.00167 0.00166 1.93812

A26 1.93818 0.00020 0.00000 0.00163 0.00163 1.93981

A27 1.88729 -0.00008 0.00000 0.00034 0.00033 1.88762

A28 1.95447 -0.00017 0.00000 -0.00019 -0.00019 1.95428

A29 1.91554 0.00006 0.00000 0.00034 0.00033 1.91587

A30 1.91553 0.00004 0.00000 0.00010 0.00010 1.91563

A31 1.90586 0.00012 0.00000 0.00119 0.00119 1.90705

A32 1.90660 0.00013 0.00000 0.00119 0.00119 1.90778

A33 1.86358 -0.00018 0.00000 -0.00273 -0.00273 1.86085

A34 1.96596 -0.00029 0.00000 -0.00079 -0.00079 1.96517

A35 1.90486 0.00016 0.00000 0.00128 0.00128 1.90614

A36 1.90671 0.00016 0.00000 0.00130 0.00130 1.90801

A37 1.91213 0.00009 0.00000 0.00041 0.00041 1.91253

A38 1.91233 0.00008 0.00000 0.00037 0.00037 1.91270

A39 1.85874 -0.00020 0.00000 -0.00267 -0.00267 1.85607

A40 1.94322 0.00017 0.00000 0.00088 0.00088 1.94410

A41 1.93954 0.00033 0.00000 0.00217 0.00217 1.94171

A42 1.93951 0.00033 0.00000 0.00213 0.00213 1.94164

A43 1.87969 -0.00028 0.00000 -0.00192 -0.00192 1.87777

A44 1.88048 -0.00028 0.00000 -0.00194 -0.00194 1.87854

A45 1.87853 -0.00032 0.00000 -0.00164 -0.00165 1.87688

D1 2.55981 0.00010 0.00000 -0.00100 -0.00100 2.55881

D2 -1.55040 -0.00004 0.00000 -0.00529 -0.00529 -1.55569

D3 0.38873 -0.00022 0.00000 -0.00718 -0.00718 0.38155

D4 -0.61563 0.00020 0.00000 0.00715 0.00715 -0.60848

D5 1.55735 0.00006 0.00000 0.00285 0.00285 1.56020

D6 -2.78670 -0.00012 0.00000 0.00096 0.00096 -2.78574

D7 -3.10843 -0.00009 0.00000 -0.00616 -0.00616 -3.11459

D8 0.00053 -0.00001 0.00000 0.00165 0.00165 0.00218

D9 -3.10758 -0.00026 0.00000 -0.00891 -0.00891 -3.11649

D10 -1.03689 -0.00017 0.00000 -0.00732 -0.00732 -1.04420

D11 1.07595 -0.00030 0.00000 -0.00963 -0.00963 1.06631

D12 1.05275 0.00009 0.00000 -0.00309 -0.00309 1.04966

D13 3.12344 0.00019 0.00000 -0.00150 -0.00150 3.12195

D14 -1.04691 0.00005 0.00000 -0.00381 -0.00381 -1.05072

D15 -0.97299 0.00003 0.00000 -0.00321 -0.00321 -0.97621

D16 1.09770 0.00013 0.00000 -0.00162 -0.00162 1.09608

D17 -3.07265 -0.00001 0.00000 -0.00394 -0.00394 -3.07659

D18 2.96398 0.00008 0.00000 0.06352 0.06352 3.02750

D19 -1.10710 0.00020 0.00000 0.06130 0.06130 -1.04580

D20 0.99003 0.00027 0.00000 0.06365 0.06365 1.05368

D21 1.84556 -0.00004 0.00000 -0.00578 -0.00577 1.83978

D22 -1.09445 -0.00036 0.00000 -0.03737 -0.03738 -1.13183

D23 2.61368 -0.00050 0.00000 -0.08314 -0.08315 2.53053

D24 -0.73170 -0.00018 0.00000 -0.05121 -0.05120 -0.78290

D25 -3.04346 0.00009 0.00000 0.03087 0.03087 -3.01258

D26 -0.92651 0.00015 0.00000 0.03112 0.03112 -0.89539

D27 1.11355 0.00003 0.00000 0.03045 0.03045 1.14400

D28 -3.12847 -0.00002 0.00000 -0.00158 -0.00158 -3.13005

D29 -1.00879 0.00006 0.00000 0.00003 0.00003 -1.00877

D30 1.03411 -0.00010 0.00000 -0.00303 -0.00303 1.03108

D31 1.07045 0.00009 0.00000 -0.00003 -0.00003 1.07042

D32 -3.09306 0.00017 0.00000 0.00158 0.00158 -3.09148

D33 -1.05016 0.00001 0.00000 -0.00148 -0.00148 -1.05163

D34 -1.02909 -0.00009 0.00000 -0.00266 -0.00266 -1.03176

D35 1.09058 -0.00001 0.00000 -0.00105 -0.00106 1.08953

D36 3.13348 -0.00017 0.00000 -0.00411 -0.00411 3.12937

D37 -3.12799 0.00001 0.00000 0.00043 0.00043 -3.12756

D38 -1.00015 0.00003 0.00000 0.00133 0.00133 -0.99882

D39 1.02578 -0.00002 0.00000 -0.00044 -0.00044 1.02535

D40 1.02996 -0.00004 0.00000 -0.00068 -0.00068 1.02927

D41 -3.12538 -0.00001 0.00000 0.00021 0.00021 -3.12517

D42 -1.09946 -0.00006 0.00000 -0.00155 -0.00155 -1.10101

D43 -1.00225 0.00003 0.00000 0.00125 0.00125 -1.00100

D44 1.12559 0.00006 0.00000 0.00215 0.00215 1.12774

D45 -3.13167 0.00001 0.00000 0.00039 0.00039 -3.13128

D46 3.13485 0.00000 0.00000 0.00006 0.00006 3.13491

D47 -1.05294 -0.00002 0.00000 -0.00032 -0.00032 -1.05327

D48 1.03848 0.00002 0.00000 0.00048 0.00048 1.03896

D49 1.01112 -0.00007 0.00000 -0.00133 -0.00133 1.00979

D50 3.10651 -0.00009 0.00000 -0.00171 -0.00171 3.10480

D51 -1.08525 -0.00005 0.00000 -0.00091 -0.00091 -1.08616

D52 -1.02210 0.00007 0.00000 0.00144 0.00144 -1.02065

D53 1.07329 0.00005 0.00000 0.00107 0.00107 1.07436

D54 -3.11847 0.00009 0.00000 0.00187 0.00187 -3.11660

Item Value Threshold Converged?

Maximum Force 0.015646 0.000450 NO

RMS Force 0.001594 0.000300 NO

Maximum Displacement 0.254590 0.001800 NO

RMS Displacement 0.082695 0.001200 NO

Predicted change in Energy=-3.037793D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:28:59 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.119610 -0.353512 -0.166287

2 6 0 -2.814611 0.023715 0.467036

3 8 0 -4.916958 0.430726 -0.634881

4 8 0 -4.325352 -1.687333 -0.199513

5 6 0 -2.364976 -0.862265 1.615387

6 16 0 -1.535739 0.052215 -0.939194

7 6 0 -0.106236 0.686735 -0.133852

8 16 0 1.125643 -0.578097 0.180893

9 16 0 -0.028305 2.280570 0.511621

10 6 0 2.708335 0.327515 -0.040492

11 6 0 3.882553 -0.644223 0.011993

12 6 0 5.226424 0.071528 -0.152407

13 6 0 6.412052 -0.891491 -0.121617

14 1 0 -2.894897 1.064245 0.777997

15 1 0 -5.176407 -1.834995 -0.645758

16 1 0 -1.422762 -0.488542 2.019816

17 1 0 -3.105788 -0.848438 2.421554

18 1 0 -2.219518 -1.894341 1.295390

19 1 0 2.666708 0.840915 -1.003944

20 1 0 2.786541 1.081452 0.743016

21 1 0 3.874661 -1.184297 0.966148

22 1 0 3.774861 -1.398369 -0.775952

23 1 0 5.227062 0.624928 -1.098839

24 1 0 5.339013 0.818653 0.641918

25 1 0 7.360492 -0.360815 -0.247325

26 1 0 6.459199 -1.432647 0.829008

27 1 0 6.339775 -1.635468 -0.921493

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.498807 0.000000

3 O 1.212590 2.408266 0.000000

4 O 1.350004 2.377880 2.241811 0.000000

5 C 2.551849 1.518500 3.639800 2.796010 0.000000

6 S 2.727341 1.901002 3.415921 3.369732 2.837215

7 C 4.146123 2.852359 4.843513 4.841637 3.249791

8 S 5.261525 3.996205 6.180310 5.575702 3.784567

9 S 4.912914 3.585928 5.351198 5.891908 4.068875

10 C 6.862977 5.554530 7.649120 7.318309 5.467723

11 C 8.009426 6.745754 8.888495 8.276624 6.453683

12 C 9.355704 8.065001 10.161201 9.712478 7.850250

13 C 10.545488 9.290609 11.417450 10.767138 8.947304

14 H 2.098006 1.088965 2.546822 3.251601 2.166444

15 H 1.881888 3.204871 2.280553 0.972231 3.736727

16 H 3.474230 2.147272 4.483512 3.845459 1.091329

17 H 2.823068 2.159995 3.776029 3.010162 1.094943

18 H 2.849737 2.172382 4.050687 2.590776 1.090292

19 H 6.941357 5.733799 7.603713 7.478506 5.922800

20 H 7.112023 5.706826 7.852766 7.689834 5.574692

21 H 8.116710 6.815773 9.080978 8.297712 6.281583

22 H 7.986619 6.854814 8.883310 8.125837 6.610862

23 H 9.443902 8.214738 10.156482 9.869344 8.198647

24 H 9.565182 8.194150 10.342420 10.019377 7.945097

25 H 11.480390 10.207394 12.309042 11.760990 9.914932

26 H 10.680184 9.394443 11.620330 10.836478 8.877487

27 H 10.564681 9.406576 11.448377 10.689662 9.099796

6 7 8 9 10

6 S 0.000000

7 C 1.759168 0.000000

8 S 2.955476 1.793430 0.000000

9 S 3.056598 1.721342 3.100477 0.000000

10 C 4.346909 2.838937 1.836861 3.407118 0.000000

11 C 5.545058 4.207512 2.762870 4.909059 1.525063

12 C 6.807809 5.368062 4.165274 5.738727 2.533541

13 C 8.045271 6.706640 5.304324 7.207022 3.900010

14 H 2.412521 2.958143 4.383898 3.125340 5.710421

15 H 4.111220 5.685754 6.479119 6.691813 8.198289

16 H 3.010137 2.784385 3.143887 3.447774 4.687940

17 H 3.817179 4.228967 4.795691 4.786381 6.422504

18 H 3.041381 3.629138 3.763603 4.779706 5.568210

19 H 4.276307 2.910335 2.406723 3.410666 1.092498

20 H 4.750922 3.048418 2.414263 3.068352 1.090148

21 H 5.867854 4.534126 2.922534 5.238802 2.158522

22 H 5.507568 4.452287 2.933727 5.445779 2.158021

23 H 6.788886 5.420248 4.461684 5.740525 2.748189

24 H 7.095742 5.501814 4.462728 5.564377 2.761769

25 H 8.932648 7.540707 6.253313 7.883352 4.707350

26 H 8.321681 6.965903 5.440324 7.481739 4.233577

27 H 8.054335 6.896671 5.433274 7.611939 4.220998

11 12 13 14 15

11 C 0.000000

12 C 1.531443 0.000000

13 C 2.545066 1.527765 0.000000

14 H 7.031319 8.234500 9.552670 0.000000

15 H 9.160531 10.587593 11.638613 3.954486 0.000000

16 H 5.674676 7.017400 8.132183 2.473953 4.796674

17 H 7.394903 8.769114 9.851845 2.530635 3.830035

18 H 6.359652 7.835995 8.804409 3.078484 3.537622

19 H 2.171645 2.805213 4.219874 5.844368 8.294772

20 H 2.171081 2.788326 4.217159 5.681571 8.593189

21 H 1.096428 2.157666 2.776206 7.135703 9.216479

22 H 1.095988 2.157879 2.764029 7.277698 8.962856

23 H 2.156942 1.096351 2.158400 8.347559 10.699938

24 H 2.158261 1.096278 2.158470 8.238696 10.921264

25 H 3.499090 2.179490 1.094056 10.404570 12.629560

26 H 2.815711 2.178405 1.094878 9.681744 11.735593

27 H 2.809253 2.178274 1.094773 9.770153 11.521210

16 17 18 19 20

16 H 0.000000

17 H 1.767341 0.000000

18 H 1.770843 1.774157 0.000000

19 H 5.256838 6.921680 6.053410 0.000000

20 H 4.670474 6.423511 5.849879 1.767509 0.000000

21 H 5.445822 7.138464 6.144232 3.072767 2.523373

22 H 5.971548 7.607220 6.361527 2.508859 3.071409

23 H 7.428727 9.165171 8.217701 2.571200 3.091439

24 H 7.023458 8.789821 8.057218 3.138562 2.567956

25 H 9.072033 10.812201 9.823862 4.903900 4.897136

26 H 8.027120 9.714240 8.703494 4.786625 4.451573

27 H 8.379959 10.050574 8.845512 4.430654 4.772601

21 22 23 24 25

21 H 0.000000

22 H 1.758038 0.000000

23 H 3.060466 2.511349 0.000000

24 H 2.502251 3.061391 1.755078 0.000000

25 H 3.781753 3.769976 2.499658 2.503652 0.000000

26 H 2.600061 3.127738 3.077071 2.521541 1.766251

27 H 3.137440 2.579958 2.525662 3.077091 1.766665

26 27

26 H 0.000000

27 H 1.766253 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 8.29D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.128732 -0.369414 -0.155883

2 6 0 -2.820909 0.042029 0.449705

3 8 0 -4.926645 0.387415 -0.666685

4 8 0 -4.336506 -1.702557 -0.110385

5 6 0 -2.368392 -0.776079 1.646271

6 16 0 -1.547097 -0.013787 -0.960293

7 6 0 -0.113779 0.664355 -0.198455

8 16 0 1.117415 -0.581949 0.185311

9 16 0 -0.031226 2.293051 0.352500

10 6 0 2.700593 0.306578 -0.094200

11 6 0 3.873598 -0.662362 0.010833

12 6 0 5.217891 0.040351 -0.199852

13 6 0 6.402240 -0.921171 -0.117027

14 1 0 -2.898577 1.099080 0.699613

15 1 0 -5.189382 -1.874641 -0.544232

16 1 0 -1.424185 -0.380913 2.024843

17 1 0 -3.106260 -0.713954 2.452863

18 1 0 -2.225574 -1.825326 1.386618

19 1 0 2.656216 0.762875 -1.085853

20 1 0 2.782716 1.104877 0.643633

21 1 0 3.868386 -1.145749 0.994939

22 1 0 3.761973 -1.461080 -0.731312

23 1 0 5.215897 0.537505 -1.177002

24 1 0 5.334426 0.832425 0.549055

25 1 0 7.350979 -0.400306 -0.276876

26 1 0 6.452051 -1.405935 0.863423

27 1 0 6.326001 -1.710493 -0.871802

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3444151 0.1912325 0.1789684

Leave Link 202 at Sat Aug 17 17:29:00 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1100.2940151255 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0547387782 Hartrees.

Nuclear repulsion after empirical dispersion term = 1100.2392763473 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2333

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.50D-11

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 104

GePol: Fraction of low-weight points (<1% of avg) = 4.46%

GePol: Cavity surface area = 309.599 Ang\*\*2

GePol: Cavity volume = 320.129 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0056876620 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1100.2335886853 Hartrees.

Leave Link 301 at Sat Aug 17 17:29:00 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:29:00 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:29:00 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999773 0.021278 0.000474 -0.000822 Ang= 2.44 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7553 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.62914234361

Leave Link 401 at Sat Aug 17 17:29:01 2019, MaxMem= 1342177280 cpu: 7.6

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16328667.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.88D-15 for 2302.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.27D-15 for 845 378.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.88D-15 for 2302.

Iteration 1 A^-1\*A deviation from orthogonality is 8.85D-08 for 1077 1035.

Iteration 2 A\*A^-1 deviation from unit magnitude is 7.33D-15 for 182.

Iteration 2 A\*A^-1 deviation from orthogonality is 4.36D-15 for 976 184.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.33D-15 for 1166.

Iteration 2 A^-1\*A deviation from orthogonality is 6.91D-16 for 2301 76.

E= -1658.66637306450

DIIS: error= 2.99D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.66637306450 IErMin= 1 ErrMin= 2.99D-03

ErrMax= 2.99D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.52D-02 BMatP= 2.52D-02

IDIUse=3 WtCom= 9.70D-01 WtEn= 2.99D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.428 Goal= None Shift= 0.000

Gap= 0.482 Goal= None Shift= 0.000

GapD= 0.428 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=3.46D-04 MaxDP=9.85D-03 OVMax= 2.11D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.45D-04 CP: 9.99D-01

E= -1658.67666042176 Delta-E= -0.010287357264 Rises=F Damp=F

DIIS: error= 6.56D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67666042176 IErMin= 2 ErrMin= 6.56D-04

ErrMax= 6.56D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.51D-04 BMatP= 2.52D-02

IDIUse=3 WtCom= 9.93D-01 WtEn= 6.56D-03

Coeff-Com: -0.447D-01 0.104D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.444D-01 0.104D+01

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=7.82D-05 MaxDP=2.46D-03 DE=-1.03D-02 OVMax= 6.13D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 7.50D-05 CP: 9.99D-01 1.06D+00

E= -1658.67664622061 Delta-E= 0.000014201154 Rises=F Damp=F

DIIS: error= 1.13D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1658.67666042176 IErMin= 2 ErrMin= 6.56D-04

ErrMax= 1.13D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.34D-04 BMatP= 5.51D-04

IDIUse=3 WtCom= 2.30D-01 WtEn= 7.70D-01

Coeff-Com: -0.416D-01 0.620D+00 0.421D+00

Coeff-En: 0.000D+00 0.526D+00 0.474D+00

Coeff: -0.956D-02 0.548D+00 0.462D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=5.04D-05 MaxDP=2.21D-03 DE= 1.42D-05 OVMax= 4.18D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 3.01D-05 CP: 9.99D-01 1.09D+00 4.79D-01

E= -1658.67680402870 Delta-E= -0.000157808094 Rises=F Damp=F

DIIS: error= 4.96D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67680402870 IErMin= 4 ErrMin= 4.96D-04

ErrMax= 4.96D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.51D-04 BMatP= 5.51D-04

IDIUse=3 WtCom= 9.95D-01 WtEn= 4.96D-03

Coeff-Com: -0.171D-01 0.216D+00 0.305D+00 0.496D+00

Coeff-En: 0.000D+00 0.000D+00 0.142D+00 0.858D+00

Coeff: -0.170D-01 0.215D+00 0.305D+00 0.498D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=1.68D-05 MaxDP=6.71D-04 DE=-1.58D-04 OVMax= 1.58D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.04D-05 CP: 9.99D-01 1.10D+00 6.08D-01 7.17D-01

E= -1658.67683160254 Delta-E= -0.000027573840 Rises=F Damp=F

DIIS: error= 9.07D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67683160254 IErMin= 5 ErrMin= 9.07D-05

ErrMax= 9.07D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.56D-06 BMatP= 1.51D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.445D-02 0.457D-01 0.124D+00 0.290D+00 0.545D+00

Coeff: -0.445D-02 0.457D-01 0.124D+00 0.290D+00 0.545D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=4.86D-06 MaxDP=2.53D-04 DE=-2.76D-05 OVMax= 4.96D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.53D-06 CP: 9.99D-01 1.10D+00 6.24D-01 8.04D-01 8.87D-01

E= -1658.67683342379 Delta-E= -0.000001821250 Rises=F Damp=F

DIIS: error= 2.47D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67683342379 IErMin= 6 ErrMin= 2.47D-05

ErrMax= 2.47D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.12D-07 BMatP= 8.56D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.284D-03-0.106D-01 0.160D-01 0.683D-01 0.260D+00 0.666D+00

Coeff: 0.284D-03-0.106D-01 0.160D-01 0.683D-01 0.260D+00 0.666D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=2.48D-06 MaxDP=1.18D-04 DE=-1.82D-06 OVMax= 3.25D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.55D-06 CP: 9.99D-01 1.11D+00 6.40D-01 8.46D-01 9.64D-01

CP: 9.87D-01

E= -1658.67683360740 Delta-E= -0.000000183604 Rises=F Damp=F

DIIS: error= 1.05D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67683360740 IErMin= 7 ErrMin= 1.05D-05

ErrMax= 1.05D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.28D-07 BMatP= 7.12D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.866D-03-0.131D-01-0.134D-01-0.159D-01 0.402D-01 0.334D+00

Coeff-Com: 0.668D+00

Coeff: 0.866D-03-0.131D-01-0.134D-01-0.159D-01 0.402D-01 0.334D+00

Coeff: 0.668D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=1.27D-06 MaxDP=5.52D-05 DE=-1.84D-07 OVMax= 1.40D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 7.77D-07 CP: 9.99D-01 1.11D+00 6.45D-01 8.64D-01 1.02D+00

CP: 1.09D+00 1.05D+00

E= -1658.67683364850 Delta-E= -0.000000041106 Rises=F Damp=F

DIIS: error= 2.24D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67683364850 IErMin= 8 ErrMin= 2.24D-06

ErrMax= 2.24D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.68D-08 BMatP= 1.28D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.313D-03-0.360D-02-0.796D-02-0.174D-01-0.216D-01 0.412D-01

Coeff-Com: 0.283D+00 0.726D+00

Coeff: 0.313D-03-0.360D-02-0.796D-02-0.174D-01-0.216D-01 0.412D-01

Coeff: 0.283D+00 0.726D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=6.31D-07 MaxDP=2.94D-05 DE=-4.11D-08 OVMax= 9.77D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.91D-07 CP: 9.99D-01 1.11D+00 6.46D-01 8.74D-01 1.04D+00

CP: 1.17D+00 1.23D+00 9.00D-01

E= -1658.67683365460 Delta-E= -0.000000006094 Rises=F Damp=F

DIIS: error= 1.93D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67683365460 IErMin= 9 ErrMin= 1.93D-06

ErrMax= 1.93D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.88D-09 BMatP= 1.68D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.192D-04 0.594D-03-0.251D-02-0.888D-02-0.250D-01-0.489D-01

Coeff-Com: 0.333D-01 0.500D+00 0.551D+00

Coeff: 0.192D-04 0.594D-03-0.251D-02-0.888D-02-0.250D-01-0.489D-01

Coeff: 0.333D-01 0.500D+00 0.551D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=2.90D-07 MaxDP=1.16D-05 DE=-6.09D-09 OVMax= 3.23D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.17D-07 CP: 9.99D-01 1.11D+00 6.48D-01 8.76D-01 1.05D+00

CP: 1.19D+00 1.29D+00 1.09D+00 7.50D-01

E= -1658.67683365748 Delta-E= -0.000000002878 Rises=F Damp=F

DIIS: error= 6.86D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67683365748 IErMin=10 ErrMin= 6.86D-07

ErrMax= 6.86D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.89D-10 BMatP= 9.88D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.405D-04 0.915D-03 0.499D-04-0.182D-02-0.906D-02-0.310D-01

Coeff-Com: -0.319D-01 0.145D+00 0.279D+00 0.648D+00

Coeff: -0.405D-04 0.915D-03 0.499D-04-0.182D-02-0.906D-02-0.310D-01

Coeff: -0.319D-01 0.145D+00 0.279D+00 0.648D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=9.50D-08 MaxDP=3.27D-06 DE=-2.88D-09 OVMax= 1.28D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 4.75D-08 CP: 9.99D-01 1.11D+00 6.48D-01 8.77D-01 1.05D+00

CP: 1.20D+00 1.31D+00 1.13D+00 8.31D-01 8.18D-01

E= -1658.67683365770 Delta-E= -0.000000000226 Rises=F Damp=F

DIIS: error= 1.95D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67683365770 IErMin=11 ErrMin= 1.95D-07

ErrMax= 1.95D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.19D-10 BMatP= 7.89D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.218D-04 0.390D-03 0.263D-03-0.110D-03-0.207D-02-0.108D-01

Coeff-Com: -0.197D-01 0.212D-01 0.772D-01 0.336D+00 0.598D+00

Coeff: -0.218D-04 0.390D-03 0.263D-03-0.110D-03-0.207D-02-0.108D-01

Coeff: -0.197D-01 0.212D-01 0.772D-01 0.336D+00 0.598D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=3.26D-08 MaxDP=1.28D-06 DE=-2.26D-10 OVMax= 3.49D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.94D-08 CP: 9.99D-01 1.11D+00 6.48D-01 8.77D-01 1.05D+00

CP: 1.20D+00 1.32D+00 1.14D+00 8.67D-01 9.37D-01

CP: 8.09D-01

E= -1658.67683365774 Delta-E= -0.000000000041 Rises=F Damp=F

DIIS: error= 6.09D-08 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.67683365774 IErMin=12 ErrMin= 6.09D-08

ErrMax= 6.09D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.14D-11 BMatP= 1.19D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.116D-07-0.441D-04 0.103D-03 0.359D-03 0.118D-02 0.263D-02

Coeff-Com: -0.800D-03-0.206D-01-0.331D-01-0.883D-02 0.222D+00 0.837D+00

Coeff: 0.116D-07-0.441D-04 0.103D-03 0.359D-03 0.118D-02 0.263D-02

Coeff: -0.800D-03-0.206D-01-0.331D-01-0.883D-02 0.222D+00 0.837D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=1.37D-08 MaxDP=7.02D-07 DE=-4.14D-11 OVMax= 1.63D-06

Cycle 13 Pass 1 IDiag 1:

RMSU= 5.72D-09 CP: 9.99D-01 1.11D+00 6.48D-01 8.77D-01 1.05D+00

CP: 1.20D+00 1.32D+00 1.14D+00 8.80D-01 9.90D-01

CP: 9.84D-01 1.01D+00

E= -1658.67683365775 Delta-E= -0.000000000009 Rises=F Damp=F

DIIS: error= 2.04D-08 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1658.67683365775 IErMin=13 ErrMin= 2.04D-08

ErrMax= 2.04D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.57D-12 BMatP= 1.14D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.256D-05-0.644D-04 0.137D-04 0.165D-03 0.723D-03 0.238D-02

Coeff-Com: 0.202D-02-0.102D-01-0.240D-01-0.427D-01 0.227D-01 0.346D+00

Coeff-Com: 0.703D+00

Coeff: 0.256D-05-0.644D-04 0.137D-04 0.165D-03 0.723D-03 0.238D-02

Coeff: 0.202D-02-0.102D-01-0.240D-01-0.427D-01 0.227D-01 0.346D+00

Coeff: 0.703D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=4.17D-09 MaxDP=1.82D-07 DE=-8.64D-12 OVMax= 4.58D-07

Error on total polarization charges = 0.04178

SCF Done: E(UB3LYP) = -1658.67683366 A.U. after 13 cycles

NFock= 13 Conv=0.42D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655234457717D+03 PE=-6.143217066864D+03 EE= 1.729072186804D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.57

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:29:29 2019, MaxMem= 1342177280 cpu: 321.1

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 343

Leave Link 701 at Sat Aug 17 17:29:30 2019, MaxMem= 1342177280 cpu: 10.3

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:29:30 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:29:33 2019, MaxMem= 1342177280 cpu: 36.0

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.36880940D+00-2.97230992D+00 4.59144900D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.002741115 0.002217705 -0.000926771

2 6 0.001431385 0.000554727 0.000552671

3 8 0.002009425 -0.001743286 0.000800929

4 8 -0.000375148 -0.000346517 -0.000410530

5 6 0.000069848 0.000532796 -0.000367062

6 16 -0.000254720 0.000177534 0.000018681

7 6 0.000277580 -0.001118087 -0.000841066

8 16 -0.000843904 0.000724627 0.000016825

9 16 0.000144384 -0.000488695 0.000576818

10 6 0.000431604 0.000097880 0.000156683

11 6 0.000125368 0.000404542 -0.000107434

12 6 0.000009115 -0.000281896 0.000163248

13 6 -0.000337435 0.000244098 -0.000030270

14 1 -0.000477067 -0.000079170 0.000304314

15 1 0.000047973 -0.000383798 -0.000029016

16 1 -0.000070163 -0.000167051 0.000042423

17 1 0.000024600 -0.000170270 0.000050710

18 1 0.000004798 -0.000102417 0.000117838

19 1 -0.000186033 -0.000086040 0.000040195

20 1 0.000350675 0.000144547 -0.000007832

21 1 0.000019576 -0.000136777 -0.000003394

22 1 -0.000064252 -0.000001300 0.000006302

23 1 -0.000017881 0.000109269 0.000049115

24 1 0.000025979 0.000063504 -0.000023360

25 1 0.000157182 -0.000119633 0.000040120

26 1 0.000118659 -0.000068968 -0.000038124

27 1 0.000119566 0.000022677 -0.000152016

-------------------------------------------------------------------

Cartesian Forces: Max 0.002741115 RMS 0.000609339

Leave Link 716 at Sat Aug 17 17:29:33 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.002771202 RMS 0.000385006

Search for a local minimum.

Step number 2 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .38501D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 1 2

DE= -1.07D-04 DEPred=-3.04D-04 R= 3.51D-01

Trust test= 3.51D-01 RLast= 1.65D-01 DXMaxT set to 3.00D-01

ITU= 0 0

Use linear search instead of GDIIS.

Eigenvalues --- 0.00172 0.00234 0.00322 0.00367 0.00400

Eigenvalues --- 0.00446 0.00487 0.00754 0.00866 0.01035

Eigenvalues --- 0.01195 0.02307 0.03510 0.03590 0.04422

Eigenvalues --- 0.04800 0.04838 0.04912 0.05059 0.05460

Eigenvalues --- 0.05478 0.05557 0.05615 0.05794 0.08223

Eigenvalues --- 0.08327 0.08625 0.11234 0.12121 0.12200

Eigenvalues --- 0.13655 0.15778 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16335 0.18429 0.19343

Eigenvalues --- 0.19709 0.21894 0.21906 0.22037 0.23407

Eigenvalues --- 0.24202 0.24886 0.24995 0.25000 0.25000

Eigenvalues --- 0.25684 0.26399 0.29130 0.29394 0.29468

Eigenvalues --- 0.29710 0.30182 0.32383 0.33256 0.33868

Eigenvalues --- 0.33879 0.33897 0.33946 0.34027 0.34033

Eigenvalues --- 0.34095 0.34189 0.34339 0.34453 0.34511

Eigenvalues --- 0.34589 0.36041 0.52336 0.56221 0.83841

RFO step: Lambda=-6.90893241D-04 EMin= 1.72391201D-03

Quartic linear search produced a step of -0.50052.

Iteration 1 RMS(Cart)= 0.20759714 RMS(Int)= 0.00837711

Iteration 2 RMS(Cart)= 0.02166666 RMS(Int)= 0.00013040

Iteration 3 RMS(Cart)= 0.00011961 RMS(Int)= 0.00012334

Iteration 4 RMS(Cart)= 0.00000002 RMS(Int)= 0.00012334

ITry= 1 IFail=0 DXMaxC= 6.21D-01 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83233 0.00123 0.00199 0.00002 0.00201 2.83434

R2 2.29146 -0.00277 0.00826 -0.01096 -0.00270 2.28876

R3 2.55114 0.00084 0.00339 -0.00286 0.00052 2.55166

R4 2.86955 -0.00023 0.00246 -0.00306 -0.00060 2.86894

R5 3.59237 0.00021 0.00394 -0.00344 0.00050 3.59287

R6 2.05785 0.00005 0.00254 -0.00267 -0.00013 2.05771

R7 1.83725 0.00001 0.00297 -0.00327 -0.00030 1.83695

R8 2.06231 -0.00008 0.00169 -0.00196 -0.00027 2.06204

R9 2.06914 0.00003 0.00181 -0.00190 -0.00009 2.06905

R10 2.06035 0.00001 0.00211 -0.00227 -0.00015 2.06020

R11 3.32435 -0.00004 0.00233 -0.00257 -0.00024 3.32411

R12 3.38909 -0.00076 0.00108 -0.00278 -0.00170 3.38739

R13 3.25287 -0.00026 0.00142 -0.00198 -0.00055 3.25231

R14 3.47116 0.00079 0.00132 0.00054 0.00186 3.47303

R15 2.88195 0.00001 0.00246 -0.00262 -0.00016 2.88179

R16 2.06452 -0.00005 0.00239 -0.00267 -0.00028 2.06424

R17 2.06008 0.00010 0.00251 -0.00255 -0.00004 2.06004

R18 2.89401 0.00003 0.00201 -0.00210 -0.00009 2.89392

R19 2.07195 0.00008 0.00181 -0.00182 -0.00001 2.07194

R20 2.07112 -0.00001 0.00188 -0.00204 -0.00016 2.07095

R21 2.88706 0.00001 0.00227 -0.00241 -0.00014 2.88692

R22 2.07180 0.00002 0.00181 -0.00193 -0.00012 2.07169

R23 2.07166 0.00002 0.00181 -0.00192 -0.00012 2.07155

R24 2.06747 0.00007 0.00189 -0.00193 -0.00004 2.06743

R25 2.06902 0.00003 0.00194 -0.00204 -0.00010 2.06892

R26 2.06882 0.00007 0.00195 -0.00199 -0.00004 2.06878

A1 2.18101 -0.00008 -0.00104 0.00077 -0.00034 2.18068

A2 1.97334 0.00005 0.00341 -0.00366 -0.00031 1.97304

A3 2.12854 0.00002 -0.00248 0.00249 -0.00005 2.12848

A4 2.01586 0.00034 -0.00072 0.00130 0.00058 2.01645

A5 1.85141 -0.00045 0.00212 -0.00322 -0.00110 1.85031

A6 1.87230 -0.00007 -0.00082 -0.00042 -0.00124 1.87106

A7 1.94869 0.00013 0.00076 0.00006 0.00083 1.94951

A8 1.94270 -0.00027 -0.00148 -0.00003 -0.00151 1.94119

A9 1.81987 0.00031 0.00032 0.00231 0.00262 1.82250

A10 1.87000 0.00079 0.00366 -0.00088 0.00278 1.87279

A11 1.91356 0.00010 -0.00217 0.00247 0.00030 1.91386

A12 1.92739 0.00008 -0.00149 0.00173 0.00024 1.92764

A13 1.94965 0.00021 0.00053 0.00031 0.00085 1.95049

A14 1.88279 -0.00010 0.00118 -0.00171 -0.00053 1.88226

A15 1.89415 -0.00013 0.00060 -0.00101 -0.00041 1.89374

A16 1.89474 -0.00017 0.00144 -0.00195 -0.00051 1.89423

A17 1.78588 0.00021 -0.00051 0.00103 0.00051 1.78639

A18 1.96506 0.00123 -0.00043 -0.00073 -0.00194 1.96311

A19 2.14412 -0.00004 -0.00116 -0.00292 -0.00487 2.13925

A20 2.16050 -0.00128 -0.00117 -0.00567 -0.00762 2.15287

A21 1.79567 0.00012 -0.00019 0.00048 0.00029 1.79595

A22 1.92316 0.00027 0.00087 -0.00001 0.00086 1.92402

A23 1.88089 -0.00029 0.00060 -0.00197 -0.00137 1.87951

A24 1.89247 0.00022 0.00040 0.00161 0.00201 1.89449

A25 1.93812 0.00006 -0.00083 0.00063 -0.00020 1.93792

A26 1.93981 -0.00030 -0.00081 -0.00003 -0.00085 1.93896

A27 1.88762 0.00004 -0.00017 -0.00026 -0.00043 1.88720

A28 1.95428 0.00009 0.00010 0.00012 0.00022 1.95449

A29 1.91587 0.00003 -0.00017 0.00030 0.00014 1.91601

A30 1.91563 -0.00009 -0.00005 -0.00024 -0.00029 1.91534

A31 1.90705 -0.00008 -0.00059 0.00017 -0.00042 1.90663

A32 1.90778 0.00006 -0.00059 0.00098 0.00038 1.90817

A33 1.86085 -0.00002 0.00137 -0.00140 -0.00003 1.86081

A34 1.96517 0.00010 0.00039 -0.00013 0.00026 1.96544

A35 1.90614 -0.00002 -0.00064 0.00053 -0.00011 1.90603

A36 1.90801 -0.00002 -0.00065 0.00062 -0.00003 1.90798

A37 1.91253 -0.00003 -0.00020 0.00012 -0.00008 1.91245

A38 1.91270 -0.00001 -0.00019 0.00030 0.00011 1.91282

A39 1.85607 -0.00003 0.00134 -0.00151 -0.00018 1.85590

A40 1.94410 0.00021 -0.00044 0.00115 0.00071 1.94481

A41 1.94171 0.00010 -0.00109 0.00148 0.00040 1.94211

A42 1.94164 0.00006 -0.00107 0.00129 0.00023 1.94187

A43 1.87777 -0.00018 0.00096 -0.00167 -0.00070 1.87707

A44 1.87854 -0.00016 0.00097 -0.00159 -0.00062 1.87792

A45 1.87688 -0.00005 0.00082 -0.00092 -0.00009 1.87679

D1 2.55881 0.00011 0.00050 0.01239 0.01289 2.57170

D2 -1.55569 0.00016 0.00265 0.01086 0.01350 -1.54219

D3 0.38155 0.00028 0.00359 0.01186 0.01545 0.39700

D4 -0.60848 -0.00018 -0.00358 -0.00501 -0.00859 -0.61707

D5 1.56020 -0.00013 -0.00143 -0.00655 -0.00798 1.55223

D6 -2.78574 -0.00001 -0.00048 -0.00555 -0.00603 -2.79177

D7 -3.11459 0.00016 0.00308 0.00879 0.01187 -3.10271

D8 0.00218 -0.00012 -0.00083 -0.00805 -0.00888 -0.00670

D9 -3.11649 -0.00005 0.00446 0.00620 0.01066 -3.10583

D10 -1.04420 -0.00006 0.00366 0.00668 0.01034 -1.03386

D11 1.06631 -0.00009 0.00482 0.00560 0.01043 1.07674

D12 1.04966 0.00020 0.00155 0.00949 0.01104 1.06069

D13 3.12195 0.00018 0.00075 0.00997 0.01072 3.13266

D14 -1.05072 0.00016 0.00191 0.00889 0.01080 -1.03992

D15 -0.97621 -0.00010 0.00161 0.00659 0.00820 -0.96800

D16 1.09608 -0.00011 0.00081 0.00708 0.00788 1.10397

D17 -3.07659 -0.00013 0.00197 0.00600 0.00797 -3.06862

D18 3.02750 0.00031 -0.03179 -0.13523 -0.16702 2.86048

D19 -1.04580 0.00050 -0.03068 -0.13584 -0.16653 -1.21232

D20 1.05368 0.00043 -0.03186 -0.13445 -0.16630 0.88738

D21 1.83978 0.00031 0.00289 0.02443 0.02737 1.86716

D22 -1.13183 0.00099 0.01871 0.08309 0.10174 -1.03009

D23 2.53053 0.00029 0.04162 0.14879 0.19028 2.72081

D24 -0.78290 -0.00026 0.02563 0.08980 0.11555 -0.66734

D25 -3.01258 -0.00008 -0.01545 -0.11134 -0.12679 -3.13938

D26 -0.89539 -0.00002 -0.01558 -0.11181 -0.12739 -1.02278

D27 1.14400 -0.00001 -0.01524 -0.11232 -0.12757 1.01643

D28 -3.13005 -0.00008 0.00079 0.00474 0.00554 -3.12452

D29 -1.00877 -0.00010 -0.00001 0.00525 0.00524 -1.00353

D30 1.03108 -0.00016 0.00152 0.00359 0.00511 1.03619

D31 1.07042 0.00007 0.00001 0.00681 0.00682 1.07724

D32 -3.09148 0.00005 -0.00079 0.00732 0.00653 -3.08495

D33 -1.05163 -0.00001 0.00074 0.00566 0.00639 -1.04524

D34 -1.03176 0.00018 0.00133 0.00674 0.00807 -1.02369

D35 1.08953 0.00016 0.00053 0.00725 0.00778 1.09730

D36 3.12937 0.00010 0.00206 0.00559 0.00764 3.13702

D37 -3.12756 0.00004 -0.00022 0.00158 0.00136 -3.12620

D38 -0.99882 0.00006 -0.00066 0.00201 0.00135 -0.99747

D39 1.02535 0.00000 0.00022 0.00084 0.00106 1.02640

D40 1.02927 0.00000 0.00034 0.00100 0.00134 1.03061

D41 -3.12517 0.00001 -0.00010 0.00143 0.00133 -3.12385

D42 -1.10101 -0.00005 0.00078 0.00026 0.00104 -1.09997

D43 -1.00100 0.00003 -0.00063 0.00203 0.00140 -0.99960

D44 1.12774 0.00005 -0.00107 0.00246 0.00139 1.12913

D45 -3.13128 -0.00001 -0.00019 0.00129 0.00110 -3.13018

D46 3.13491 0.00002 -0.00003 0.00286 0.00283 3.13774

D47 -1.05327 0.00000 0.00016 0.00252 0.00268 -1.05058

D48 1.03896 0.00004 -0.00024 0.00323 0.00299 1.04195

D49 1.00979 0.00000 0.00067 0.00219 0.00286 1.01265

D50 3.10480 -0.00002 0.00086 0.00186 0.00271 3.10751

D51 -1.08616 0.00002 0.00045 0.00256 0.00301 -1.08314

D52 -1.02065 0.00005 -0.00072 0.00378 0.00305 -1.01760

D53 1.07436 0.00003 -0.00053 0.00344 0.00291 1.07727

D54 -3.11660 0.00007 -0.00093 0.00414 0.00321 -3.11339

Item Value Threshold Converged?

Maximum Force 0.002771 0.000450 NO

RMS Force 0.000385 0.000300 NO

Maximum Displacement 0.620875 0.001800 NO

RMS Displacement 0.210379 0.001200 NO

Predicted change in Energy=-3.641248D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:29:33 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.157837 -0.200061 -0.007591

2 6 0 -2.761967 -0.031573 0.514682

3 8 0 -4.870912 0.703113 -0.385361

4 8 0 -4.544391 -1.492034 -0.075719

5 6 0 -2.340296 -1.020976 1.586197

6 16 0 -1.620612 -0.111013 -1.003807

7 6 0 -0.118012 0.558318 -0.380576

8 16 0 1.143015 -0.693193 -0.142469

9 16 0 -0.013736 2.144205 0.279802

10 6 0 2.703272 0.273600 -0.235147

11 6 0 3.905649 -0.646623 -0.053371

12 6 0 5.228786 0.123007 -0.099786

13 6 0 6.444374 -0.788493 0.059444

14 1 0 -2.672009 0.994410 0.868176

15 1 0 -5.439307 -1.506442 -0.454983

16 1 0 -1.327886 -0.789817 1.921281

17 1 0 -3.004845 -0.951688 2.453588

18 1 0 -2.357060 -2.046969 1.217940

19 1 0 2.730748 0.766785 -1.209436

20 1 0 2.679526 1.044867 0.534891

21 1 0 3.827787 -1.173947 0.904757

22 1 0 3.905277 -1.414907 -0.834868

23 1 0 5.297828 0.664621 -1.050437

24 1 0 5.233743 0.883708 0.689517

25 1 0 7.378239 -0.219968 0.019565

26 1 0 6.421001 -1.318122 1.017354

27 1 0 6.481784 -1.542446 -0.733420

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.499870 0.000000

3 O 1.211161 2.407797 0.000000

4 O 1.350281 2.378771 2.240796 0.000000

5 C 2.552943 1.518180 3.641915 2.800339 0.000000

6 S 2.727249 1.901266 3.407304 3.364082 2.837975

7 C 4.127281 2.853062 4.755108 4.887710 3.361683

8 S 5.325449 4.014783 6.178672 5.743622 3.902459

9 S 4.769880 3.513112 5.109926 5.820263 4.139797

10 C 6.881203 5.524872 7.587839 7.461333 5.516411

11 C 8.075972 6.719976 8.885945 8.492255 6.468396

12 C 9.392633 8.015835 10.120374 9.905752 7.838509

13 C 10.618739 9.248616 11.421840 11.012093 8.919386

14 H 2.097955 1.088895 2.547819 3.252562 2.165033

15 H 1.883867 3.206811 2.282554 0.972072 3.742455

16 H 3.475195 2.147101 4.483578 3.850587 1.091187

17 H 2.819882 2.159852 3.778916 3.009912 1.094894

18 H 2.855835 2.172635 4.056227 2.601139 1.090210

19 H 7.059166 5.812047 7.646462 7.701638 6.060292

20 H 6.970916 5.546980 7.613986 7.680735 5.529156

21 H 8.096359 6.699406 8.991948 8.435394 6.207496

22 H 8.195977 6.941689 9.039333 8.484052 6.709986

23 H 9.552214 8.239817 10.190538 10.122771 8.254332

24 H 9.479572 8.049825 10.163268 10.091661 7.861165

25 H 11.536125 10.154034 12.290554 11.990676 9.876530

26 H 10.687019 9.286269 11.556829 11.021110 8.784771

27 H 10.748505 9.449203 11.577883 11.045887 9.136829

6 7 8 9 10

6 S 0.000000

7 C 1.759042 0.000000

8 S 2.952706 1.792530 0.000000

9 S 3.052165 1.721049 3.093092 0.000000

10 C 4.408485 2.839340 1.837846 3.338632 0.000000

11 C 5.632918 4.212931 2.764462 4.822997 1.524980

12 C 6.912761 5.371832 4.166716 5.631462 2.533618

13 C 8.162934 6.713600 5.306058 7.096228 3.900086

14 H 2.414895 2.876188 4.292298 2.955441 5.534486

15 H 4.102543 5.708323 6.639729 6.580574 8.337773

16 H 3.017053 2.929131 3.220831 3.609699 4.693748

17 H 3.817908 4.318149 4.900110 4.822514 6.427537

18 H 3.037506 3.788946 3.991735 4.892567 5.753561

19 H 4.443776 2.974206 2.406419 3.412815 1.092349

20 H 4.711140 2.983459 2.416720 2.920150 1.090126

21 H 5.870051 4.496905 2.921610 5.114489 2.158543

22 H 5.680152 4.504092 2.937750 5.410030 2.157670

23 H 6.961939 5.458143 4.464362 5.671985 2.747602

24 H 7.130147 5.467380 4.462384 5.412277 2.762339

25 H 9.057509 7.547159 6.255254 7.765199 4.707845

26 H 8.379126 6.945064 5.439932 7.344217 4.233657

27 H 8.232310 6.935056 5.438097 7.537227 4.221783

11 12 13 14 15

11 C 0.000000

12 C 1.531397 0.000000

13 C 2.545188 1.527692 0.000000

14 H 6.841624 8.007425 9.324228 0.000000

15 H 9.393018 10.797660 11.916457 3.957645 0.000000

16 H 5.595502 6.921554 7.992150 2.469648 4.802496

17 H 7.357502 8.687196 9.749169 2.532116 3.833294

18 H 6.542073 7.999391 8.966109 3.077583 3.548392

19 H 2.171313 2.808196 4.221370 5.792933 8.513904

20 H 2.170384 2.784127 4.214420 5.362141 8.567642

21 H 1.096422 2.157312 2.776627 6.852041 9.372219

22 H 1.095901 2.158055 2.763911 7.208735 9.352750

23 H 2.156771 1.096289 2.158227 8.204154 10.970603

24 H 2.158154 1.096216 2.158443 7.908545 10.997121

25 H 3.499462 2.179914 1.094036 10.158855 12.890682

26 H 2.815024 2.178585 1.094826 9.383650 11.952830

27 H 2.810949 2.178355 1.094750 9.632895 11.924396

16 17 18 19 20

16 H 0.000000

17 H 1.766846 0.000000

18 H 1.770402 1.773723 0.000000

19 H 5.356950 7.019112 6.300410 0.000000

20 H 4.620335 6.322951 5.949219 1.767097 0.000000

21 H 5.268951 7.009504 6.254006 3.072418 2.525557

22 H 5.947528 7.666701 6.620452 2.505913 3.070699

23 H 7.405848 9.155601 8.431818 2.574027 3.084373

24 H 6.882797 8.622932 8.154041 3.143990 2.563962

25 H 8.929605 10.689636 9.977478 4.907473 4.893185

26 H 7.819299 9.541678 8.810551 4.787839 4.451418

27 H 8.282803 10.025076 9.065732 4.430509 4.770740

21 22 23 24 25

21 H 0.000000

22 H 1.757943 0.000000

23 H 3.060087 2.511992 0.000000

24 H 2.501396 3.061406 1.754864 0.000000

25 H 3.781447 3.770862 2.501102 2.503158 0.000000

26 H 2.599658 3.125534 3.077100 2.522918 1.765737

27 H 3.140559 2.581656 2.524559 3.077106 1.766230

26 27

26 H 0.000000

27 H 1.766133 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.75D-01

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.152497 -0.197439 -0.017720

2 6 0 -2.760760 -0.059247 0.524111

3 8 0 -4.865803 0.726307 -0.341444

4 8 0 -4.534526 -1.483359 -0.171744

5 6 0 -2.343314 -1.114582 1.532514

6 16 0 -1.608822 -0.037485 -0.988297

7 6 0 -0.112616 0.594277 -0.312669

8 16 0 1.150672 -0.666596 -0.146937

9 16 0 -0.017821 2.134529 0.449334

10 6 0 2.708487 0.308352 -0.166120

11 6 0 3.912474 -0.618447 -0.035644

12 6 0 5.233478 0.156126 -0.023043

13 6 0 6.450802 -0.760478 0.085590

14 1 0 -2.676433 0.942031 0.943664

15 1 0 -5.426782 -1.475672 -0.557415

16 1 0 -1.333945 -0.902804 1.888902

17 1 0 -3.013983 -1.103187 2.397885

18 1 0 -2.354349 -2.114721 1.098741

19 1 0 2.741068 0.863440 -1.106356

20 1 0 2.677069 1.028265 0.651873

21 1 0 3.829726 -1.206695 0.885908

22 1 0 3.919844 -1.334709 -0.865050

23 1 0 5.307310 0.758128 -0.936274

24 1 0 5.230662 0.864330 0.813695

25 1 0 7.383130 -0.188057 0.089014

26 1 0 6.422550 -1.350866 1.007158

27 1 0 6.495985 -1.461604 -0.753969

---------------------------------------------------------------------

Rotational constants (GHZ): 1.4527110 0.1886792 0.1777538

Leave Link 202 at Sat Aug 17 17:29:33 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1100.3842080992 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0546544553 Hartrees.

Nuclear repulsion after empirical dispersion term = 1100.3295536440 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2344

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.62D-11

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 80

GePol: Fraction of low-weight points (<1% of avg) = 3.41%

GePol: Cavity surface area = 309.123 Ang\*\*2

GePol: Cavity volume = 319.940 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0054327320 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1100.3241209119 Hartrees.

Leave Link 301 at Sat Aug 17 17:29:33 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.86D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 290 291 291 291 291 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:29:33 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:29:33 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.998892 -0.047019 -0.000904 0.001748 Ang= -5.39 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7551 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.62950270150

Leave Link 401 at Sat Aug 17 17:29:34 2019, MaxMem= 1342177280 cpu: 7.5

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16483008.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.33D-15 for 2336.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.40D-15 for 705 440.

Iteration 1 A^-1\*A deviation from unit magnitude is 4.77D-15 for 2336.

Iteration 1 A^-1\*A deviation from orthogonality is 1.01D-10 for 1598 1452.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.55D-15 for 395.

Iteration 2 A\*A^-1 deviation from orthogonality is 3.28D-15 for 697 303.

Iteration 2 A^-1\*A deviation from unit magnitude is 9.99D-16 for 1244.

Iteration 2 A^-1\*A deviation from orthogonality is 3.00D-16 for 2296 2213.

E= -1658.61325448213

DIIS: error= 9.20D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.61325448213 IErMin= 1 ErrMin= 9.20D-03

ErrMax= 9.20D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.51D-01 BMatP= 1.51D-01

IDIUse=3 WtCom= 9.08D-01 WtEn= 9.20D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.426 Goal= None Shift= 0.000

Gap= 0.486 Goal= None Shift= 0.000

GapD= 0.426 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=8.53D-04 MaxDP=2.39D-02 OVMax= 5.05D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 8.52D-04 CP: 9.98D-01

E= -1658.67545838839 Delta-E= -0.062203906263 Rises=F Damp=F

DIIS: error= 1.04D-03 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67545838839 IErMin= 2 ErrMin= 1.04D-03

ErrMax= 1.04D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.80D-03 BMatP= 1.51D-01

IDIUse=3 WtCom= 9.90D-01 WtEn= 1.04D-02

Coeff-Com: -0.516D-01 0.105D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.511D-01 0.105D+01

Gap= 0.119 Goal= None Shift= 0.000

Gap= 0.138 Goal= None Shift= 0.000

RMSDP=1.99D-04 MaxDP=1.16D-02 DE=-6.22D-02 OVMax= 1.57D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.94D-04 CP: 9.97D-01 1.05D+00

E= -1658.67523589115 Delta-E= 0.000222497244 Rises=F Damp=F

DIIS: error= 2.38D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1658.67545838839 IErMin= 2 ErrMin= 1.04D-03

ErrMax= 2.38D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.59D-03 BMatP= 2.80D-03

IDIUse=3 WtCom= 1.70D-01 WtEn= 8.30D-01

Coeff-Com: -0.436D-01 0.655D+00 0.389D+00

Coeff-En: 0.000D+00 0.570D+00 0.430D+00

Coeff: -0.742D-02 0.585D+00 0.423D+00

Gap= 0.116 Goal= None Shift= 0.000

Gap= 0.139 Goal= None Shift= 0.000

RMSDP=1.39D-04 MaxDP=9.02D-03 DE= 2.22D-04 OVMax= 1.18D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 7.49D-05 CP: 9.98D-01 1.09D+00 4.15D-01

E= -1658.67623760215 Delta-E= -0.001001711002 Rises=F Damp=F

DIIS: error= 9.54D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67623760215 IErMin= 4 ErrMin= 9.54D-04

ErrMax= 9.54D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.86D-04 BMatP= 2.80D-03

IDIUse=3 WtCom= 9.90D-01 WtEn= 9.54D-03

Coeff-Com: -0.128D-01 0.154D+00 0.282D+00 0.577D+00

Coeff-En: 0.000D+00 0.000D+00 0.147D+00 0.853D+00

Coeff: -0.127D-01 0.152D+00 0.281D+00 0.580D+00

Gap= 0.117 Goal= None Shift= 0.000

Gap= 0.139 Goal= None Shift= 0.000

RMSDP=3.98D-05 MaxDP=1.56D-03 DE=-1.00D-03 OVMax= 3.24D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.39D-05 CP: 9.98D-01 1.10D+00 5.49D-01 7.83D-01

E= -1658.67639509154 Delta-E= -0.000157489392 Rises=F Damp=F

DIIS: error= 1.08D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67639509154 IErMin= 5 ErrMin= 1.08D-04

ErrMax= 1.08D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.66D-05 BMatP= 7.86D-04

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.08D-03

Coeff-Com: -0.298D-02 0.255D-01 0.100D+00 0.258D+00 0.619D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.297D-02 0.254D-01 0.100D+00 0.258D+00 0.620D+00

Gap= 0.117 Goal= None Shift= 0.000

Gap= 0.139 Goal= None Shift= 0.000

RMSDP=1.06D-05 MaxDP=5.24D-04 DE=-1.57D-04 OVMax= 9.70D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 8.10D-06 CP: 9.98D-01 1.10D+00 5.78D-01 8.29D-01 9.30D-01

E= -1658.67639889607 Delta-E= -0.000003804526 Rises=F Damp=F

DIIS: error= 5.44D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67639889607 IErMin= 6 ErrMin= 5.44D-05

ErrMax= 5.44D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.08D-06 BMatP= 1.66D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.825D-03-0.170D-01 0.124D-02 0.324D-01 0.349D+00 0.633D+00

Coeff: 0.825D-03-0.170D-01 0.124D-02 0.324D-01 0.349D+00 0.633D+00

Gap= 0.117 Goal= None Shift= 0.000

Gap= 0.139 Goal= None Shift= 0.000

RMSDP=6.13D-06 MaxDP=2.97D-04 DE=-3.80D-06 OVMax= 8.00D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 3.65D-06 CP: 9.98D-01 1.10D+00 5.82D-01 8.84D-01 1.02D+00

CP: 8.72D-01

E= -1658.67640000778 Delta-E= -0.000001111711 Rises=F Damp=F

DIIS: error= 1.93D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67640000778 IErMin= 7 ErrMin= 1.93D-05

ErrMax= 1.93D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.67D-07 BMatP= 4.08D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.850D-03-0.127D-01-0.128D-01-0.182D-01 0.101D+00 0.342D+00

Coeff-Com: 0.600D+00

Coeff: 0.850D-03-0.127D-01-0.128D-01-0.182D-01 0.101D+00 0.342D+00

Coeff: 0.600D+00

Gap= 0.117 Goal= None Shift= 0.000

Gap= 0.139 Goal= None Shift= 0.000

RMSDP=2.69D-06 MaxDP=1.14D-04 DE=-1.11D-06 OVMax= 2.75D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.81D-06 CP: 9.98D-01 1.10D+00 5.87D-01 8.90D-01 1.07D+00

CP: 9.87D-01 9.80D-01

E= -1658.67640020661 Delta-E= -0.000000198829 Rises=F Damp=F

DIIS: error= 8.25D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67640020661 IErMin= 8 ErrMin= 8.25D-06

ErrMax= 8.25D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.51D-07 BMatP= 6.67D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.262D-03-0.254D-02-0.741D-02-0.189D-01-0.305D-01 0.360D-01

Coeff-Com: 0.349D+00 0.674D+00

Coeff: 0.262D-03-0.254D-02-0.741D-02-0.189D-01-0.305D-01 0.360D-01

Coeff: 0.349D+00 0.674D+00

Gap= 0.117 Goal= None Shift= 0.000

Gap= 0.139 Goal= None Shift= 0.000

RMSDP=1.47D-06 MaxDP=6.52D-05 DE=-1.99D-07 OVMax= 2.28D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 5.83D-07 CP: 9.98D-01 1.10D+00 5.88D-01 8.99D-01 1.10D+00

CP: 1.07D+00 1.16D+00 8.04D-01

E= -1658.67640026223 Delta-E= -0.000000055617 Rises=F Damp=F

DIIS: error= 2.60D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67640026223 IErMin= 9 ErrMin= 2.60D-06

ErrMax= 2.60D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.50D-08 BMatP= 1.51D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.114D-04 0.929D-03-0.175D-02-0.722D-02-0.342D-01-0.406D-01

Coeff-Com: 0.672D-01 0.354D+00 0.662D+00

Coeff: -0.114D-04 0.929D-03-0.175D-02-0.722D-02-0.342D-01-0.406D-01

Coeff: 0.672D-01 0.354D+00 0.662D+00

Gap= 0.117 Goal= None Shift= 0.000

Gap= 0.139 Goal= None Shift= 0.000

RMSDP=5.80D-07 MaxDP=2.41D-05 DE=-5.56D-08 OVMax= 6.75D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 2.30D-07 CP: 9.98D-01 1.10D+00 5.89D-01 9.02D-01 1.11D+00

CP: 1.09D+00 1.23D+00 9.36D-01 8.71D-01

E= -1658.67640026986 Delta-E= -0.000000007636 Rises=F Damp=F

DIIS: error= 1.30D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67640026986 IErMin=10 ErrMin= 1.30D-06

ErrMax= 1.30D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.85D-09 BMatP= 2.50D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.393D-04 0.830D-03 0.120D-03-0.122D-02-0.137D-01-0.263D-01

Coeff-Com: -0.187D-01 0.962D-01 0.355D+00 0.608D+00

Coeff: -0.393D-04 0.830D-03 0.120D-03-0.122D-02-0.137D-01-0.263D-01

Coeff: -0.187D-01 0.962D-01 0.355D+00 0.608D+00

Gap= 0.117 Goal= None Shift= 0.000

Gap= 0.139 Goal= None Shift= 0.000

RMSDP=1.66D-07 MaxDP=7.08D-06 DE=-7.64D-09 OVMax= 2.46D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 8.29D-08 CP: 9.98D-01 1.10D+00 5.89D-01 9.03D-01 1.11D+00

CP: 1.10D+00 1.25D+00 9.67D-01 9.73D-01 8.76D-01

E= -1658.67640027091 Delta-E= -0.000000001050 Rises=F Damp=F

DIIS: error= 2.79D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67640027091 IErMin=11 ErrMin= 2.79D-07

ErrMax= 2.79D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.13D-10 BMatP= 3.85D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.120D-04 0.186D-03 0.200D-03 0.213D-03-0.139D-02-0.469D-02

Coeff-Com: -0.131D-01 0.268D-02 0.519D-01 0.212D+00 0.752D+00

Coeff: -0.120D-04 0.186D-03 0.200D-03 0.213D-03-0.139D-02-0.469D-02

Coeff: -0.131D-01 0.268D-02 0.519D-01 0.212D+00 0.752D+00

Gap= 0.117 Goal= None Shift= 0.000

Gap= 0.139 Goal= None Shift= 0.000

RMSDP=5.37D-08 MaxDP=2.26D-06 DE=-1.05D-09 OVMax= 6.26D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 3.07D-08 CP: 9.98D-01 1.10D+00 5.89D-01 9.02D-01 1.11D+00

CP: 1.10D+00 1.25D+00 9.76D-01 1.01D+00 9.69D-01

CP: 1.09D+00

E= -1658.67640027097 Delta-E= -0.000000000055 Rises=F Damp=F

DIIS: error= 1.49D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.67640027097 IErMin=12 ErrMin= 1.49D-07

ErrMax= 1.49D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.26D-11 BMatP= 2.13D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.169D-05-0.728D-04 0.866D-04 0.367D-03 0.215D-02 0.302D-02

Coeff-Com: -0.322D-02-0.179D-01-0.489D-01-0.935D-02 0.403D+00 0.670D+00

Coeff: 0.169D-05-0.728D-04 0.866D-04 0.367D-03 0.215D-02 0.302D-02

Coeff: -0.322D-02-0.179D-01-0.489D-01-0.935D-02 0.403D+00 0.670D+00

Gap= 0.117 Goal= None Shift= 0.000

Gap= 0.139 Goal= None Shift= 0.000

RMSDP=2.64D-08 MaxDP=1.39D-06 DE=-5.46D-11 OVMax= 3.30D-06

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.16D-08 CP: 9.98D-01 1.10D+00 5.89D-01 9.02D-01 1.11D+00

CP: 1.10D+00 1.26D+00 9.79D-01 1.02D+00 1.03D+00

CP: 1.25D+00 8.98D-01

E= -1658.67640027098 Delta-E= -0.000000000011 Rises=F Damp=F

DIIS: error= 3.65D-08 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1658.67640027098 IErMin=13 ErrMin= 3.65D-08

ErrMax= 3.65D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.14D-12 BMatP= 6.26D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.213D-05-0.490D-04 0.369D-05 0.925D-04 0.911D-03 0.164D-02

Coeff-Com: 0.750D-03-0.586D-02-0.247D-01-0.308D-01 0.380D-01 0.221D+00

Coeff-Com: 0.799D+00

Coeff: 0.213D-05-0.490D-04 0.369D-05 0.925D-04 0.911D-03 0.164D-02

Coeff: 0.750D-03-0.586D-02-0.247D-01-0.308D-01 0.380D-01 0.221D+00

Coeff: 0.799D+00

Gap= 0.117 Goal= None Shift= 0.000

Gap= 0.139 Goal= None Shift= 0.000

RMSDP=9.32D-09 MaxDP=3.47D-07 DE=-1.09D-11 OVMax= 1.12D-06

Error on total polarization charges = 0.04179

SCF Done: E(UB3LYP) = -1658.67640027 A.U. after 13 cycles

NFock= 13 Conv=0.93D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655247193464D+03 PE=-6.143467783535D+03 EE= 1.729220068889D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.41

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:30:02 2019, MaxMem= 1342177280 cpu: 322.7

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 342

Leave Link 701 at Sat Aug 17 17:30:03 2019, MaxMem= 1342177280 cpu: 10.3

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:30:03 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:30:06 2019, MaxMem= 1342177280 cpu: 36.0

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.35104718D+00-2.86529743D+00 4.34003721D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000483357 0.001573525 -0.002511686

2 6 0.000104110 -0.001753104 0.000255725

3 8 0.000184092 -0.000444541 0.000941423

4 8 -0.000321307 -0.000869004 0.000680653

5 6 0.000297439 0.000476241 -0.000189233

6 16 -0.000298220 0.000952911 0.000176458

7 6 -0.000457057 0.000741029 0.000617227

8 16 0.000602173 -0.000821325 0.001406111

9 16 -0.000173122 0.001346057 0.000045281

10 6 -0.000057137 -0.000682411 -0.000619038

11 6 -0.000053759 0.000013924 -0.000295015

12 6 -0.000053370 -0.000390944 -0.000157398

13 6 -0.000026878 -0.000017109 -0.000040388

14 1 0.000379338 0.000460305 -0.000864765

15 1 -0.000066335 -0.000221158 -0.000062235

16 1 0.000449402 0.000021009 0.000023543

17 1 0.000124249 -0.000254594 0.000408887

18 1 -0.000032154 -0.000104922 0.000208387

19 1 0.000249270 0.000383734 -0.000006446

20 1 -0.000658874 -0.000393581 0.000049746

21 1 -0.000046549 0.000053156 -0.000085340

22 1 0.000257286 -0.000244712 -0.000005231

23 1 0.000053784 0.000100382 -0.000026924

24 1 -0.000094212 0.000065963 0.000015776

25 1 0.000106506 0.000077502 -0.000013258

26 1 0.000024074 -0.000020749 0.000107063

27 1 -0.000009391 -0.000047584 -0.000059326

-------------------------------------------------------------------

Cartesian Forces: Max 0.002511686 RMS 0.000564134

Leave Link 716 at Sat Aug 17 17:30:06 2019, MaxMem= 1342177280 cpu: 0.3

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.003354963 RMS 0.000602546

Search for a local minimum.

Step number 3 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .60255D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3

DE= 4.33D-04 DEPred=-3.64D-04 R=-1.19D+00

Trust test=-1.19D+00 RLast= 4.42D-01 DXMaxT set to 1.50D-01

ITU= -1 0 0

Eigenvalues --- 0.00201 0.00237 0.00322 0.00367 0.00399

Eigenvalues --- 0.00443 0.00486 0.00753 0.01020 0.01072

Eigenvalues --- 0.01530 0.02308 0.03509 0.03589 0.04420

Eigenvalues --- 0.04790 0.04837 0.04915 0.05285 0.05455

Eigenvalues --- 0.05472 0.05560 0.05621 0.05792 0.08231

Eigenvalues --- 0.08330 0.08621 0.11231 0.12137 0.12203

Eigenvalues --- 0.13816 0.15294 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16035 0.16392 0.18454 0.18857

Eigenvalues --- 0.19715 0.21894 0.21915 0.22038 0.23397

Eigenvalues --- 0.23980 0.24831 0.24985 0.25000 0.25217

Eigenvalues --- 0.26204 0.28814 0.28943 0.29299 0.29404

Eigenvalues --- 0.29632 0.30220 0.32014 0.33602 0.33876

Eigenvalues --- 0.33881 0.33904 0.33944 0.34027 0.34038

Eigenvalues --- 0.34095 0.34187 0.34350 0.34506 0.34541

Eigenvalues --- 0.34582 0.35593 0.51714 0.56373 0.71368

En-DIIS/RFO-DIIS IScMMF= 0 using points: 3 2

RFO step: Lambda=-1.70594849D-04.

NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=T DC= -4.33D-04 SmlDif= 1.00D-05

RMS Error= 0.3742680648D-02 NUsed= 2 EDIIS=F

DidBck=T Rises=T RFO-DIIS coefs: -0.01228 1.01228

Iteration 1 RMS(Cart)= 0.23151677 RMS(Int)= 0.03537759

Iteration 2 RMS(Cart)= 0.16031818 RMS(Int)= 0.00681712

Iteration 3 RMS(Cart)= 0.01772951 RMS(Int)= 0.00012781

Iteration 4 RMS(Cart)= 0.00014569 RMS(Int)= 0.00011357

Iteration 5 RMS(Cart)= 0.00000001 RMS(Int)= 0.00011357

ITry= 1 IFail=0 DXMaxC= 1.31D+00 DCOld= 1.00D+10 DXMaxT= 1.50D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83434 0.00098 -0.00203 0.00096 -0.00107 2.83327

R2 2.28876 -0.00073 0.00273 -0.01811 -0.01537 2.27339

R3 2.55166 0.00112 -0.00053 -0.00416 -0.00469 2.54698

R4 2.86894 0.00047 0.00061 -0.00519 -0.00458 2.86437

R5 3.59287 -0.00139 -0.00051 -0.00593 -0.00643 3.58644

R6 2.05771 0.00018 0.00013 -0.00433 -0.00420 2.05352

R7 1.83695 0.00010 0.00031 -0.00525 -0.00494 1.83201

R8 2.06204 0.00042 0.00027 -0.00323 -0.00296 2.05908

R9 2.06905 0.00022 0.00009 -0.00308 -0.00299 2.06606

R10 2.06020 0.00005 0.00016 -0.00371 -0.00355 2.05665

R11 3.32411 0.00018 0.00024 -0.00426 -0.00402 3.32008

R12 3.38739 0.00154 0.00172 -0.00509 -0.00336 3.38403

R13 3.25231 0.00125 0.00056 -0.00332 -0.00276 3.24955

R14 3.47303 -0.00074 -0.00189 0.00150 -0.00038 3.47264

R15 2.88179 0.00028 0.00016 -0.00431 -0.00415 2.87765

R16 2.06424 0.00018 0.00028 -0.00440 -0.00411 2.06013

R17 2.06004 -0.00022 0.00004 -0.00414 -0.00410 2.05594

R18 2.89392 -0.00009 0.00009 -0.00347 -0.00338 2.89054

R19 2.07194 -0.00010 0.00001 -0.00295 -0.00294 2.06900

R20 2.07095 0.00017 0.00017 -0.00334 -0.00318 2.06778

R21 2.88692 0.00007 0.00014 -0.00398 -0.00384 2.88308

R22 2.07169 0.00007 0.00012 -0.00315 -0.00304 2.06865

R23 2.07155 0.00007 0.00012 -0.00314 -0.00303 2.06852

R24 2.06743 0.00014 0.00004 -0.00311 -0.00307 2.06435

R25 2.06892 0.00010 0.00010 -0.00331 -0.00321 2.06571

R26 2.06878 0.00007 0.00004 -0.00321 -0.00317 2.06561

A1 2.18068 0.00022 0.00034 0.00117 0.00158 2.18226

A2 1.97304 -0.00052 0.00031 -0.00624 -0.00586 1.96718

A3 2.12848 0.00033 0.00005 0.00414 0.00426 2.13274

A4 2.01645 0.00063 -0.00059 0.00234 0.00174 2.01818

A5 1.85031 0.00035 0.00111 -0.00671 -0.00559 1.84472

A6 1.87106 -0.00011 0.00126 -0.00003 0.00122 1.87228

A7 1.94951 -0.00063 -0.00084 -0.00047 -0.00131 1.94820

A8 1.94119 0.00011 0.00153 0.00062 0.00214 1.94333

A9 1.82250 -0.00042 -0.00266 0.00423 0.00158 1.82407

A10 1.87279 0.00039 -0.00282 -0.00068 -0.00350 1.86929

A11 1.91386 -0.00016 -0.00030 0.00458 0.00428 1.91814

A12 1.92764 0.00063 -0.00025 0.00315 0.00290 1.93054

A13 1.95049 0.00016 -0.00086 0.00069 -0.00017 1.95033

A14 1.88226 -0.00019 0.00054 -0.00293 -0.00240 1.87986

A15 1.89374 -0.00010 0.00041 -0.00180 -0.00139 1.89235

A16 1.89423 -0.00037 0.00052 -0.00399 -0.00347 1.89076

A17 1.78639 -0.00023 -0.00052 0.00187 0.00135 1.78774

A18 1.96311 -0.00335 0.00197 0.00131 0.00399 1.96710

A19 2.13925 0.00126 0.00493 -0.00289 0.00277 2.14202

A20 2.15287 0.00217 0.00772 -0.00848 -0.00005 2.15282

A21 1.79595 0.00156 -0.00029 0.00108 0.00079 1.79674

A22 1.92402 0.00008 -0.00087 0.00017 -0.00070 1.92332

A23 1.87951 0.00038 0.00139 -0.00405 -0.00266 1.87685

A24 1.89449 -0.00071 -0.00204 0.00302 0.00098 1.89547

A25 1.93792 -0.00035 0.00021 0.00108 0.00129 1.93920

A26 1.93896 0.00064 0.00086 -0.00006 0.00080 1.93976

A27 1.88720 -0.00006 0.00043 -0.00023 0.00020 1.88740

A28 1.95449 -0.00004 -0.00022 0.00055 0.00033 1.95482

A29 1.91601 -0.00008 -0.00014 0.00063 0.00049 1.91649

A30 1.91534 0.00026 0.00030 -0.00041 -0.00011 1.91523

A31 1.90663 0.00009 0.00043 0.00039 0.00082 1.90744

A32 1.90817 -0.00017 -0.00039 0.00195 0.00157 1.90973

A33 1.86081 -0.00004 0.00003 -0.00329 -0.00325 1.85756

A34 1.96544 0.00019 -0.00026 0.00015 -0.00012 1.96532

A35 1.90603 0.00001 0.00011 0.00107 0.00118 1.90721

A36 1.90798 -0.00014 0.00003 0.00121 0.00124 1.90922

A37 1.91245 -0.00009 0.00009 0.00022 0.00031 1.91276

A38 1.91282 0.00002 -0.00012 0.00061 0.00049 1.91331

A39 1.85590 0.00000 0.00018 -0.00347 -0.00329 1.85260

A40 1.94481 -0.00003 -0.00071 0.00214 0.00142 1.94623

A41 1.94211 0.00002 -0.00040 0.00276 0.00236 1.94447

A42 1.94187 -0.00002 -0.00023 0.00237 0.00214 1.94401

A43 1.87707 -0.00001 0.00071 -0.00320 -0.00249 1.87458

A44 1.87792 0.00002 0.00063 -0.00305 -0.00242 1.87550

A45 1.87679 0.00002 0.00009 -0.00150 -0.00141 1.87538

D1 2.57170 -0.00013 -0.01305 0.01878 0.00573 2.57743

D2 -1.54219 -0.00026 -0.01367 0.01455 0.00088 -1.54131

D3 0.39700 -0.00064 -0.01564 0.01635 0.00071 0.39771

D4 -0.61707 0.00057 0.00869 -0.00325 0.00544 -0.61163

D5 1.55223 0.00044 0.00807 -0.00748 0.00059 1.55282

D6 -2.79177 0.00006 0.00610 -0.00568 0.00042 -2.79136

D7 -3.10271 -0.00028 -0.01202 0.01001 -0.00201 -3.10472

D8 -0.00670 0.00040 0.00899 -0.01135 -0.00236 -0.00906

D9 -3.10583 -0.00012 -0.01079 -0.00671 -0.01751 -3.12334

D10 -1.03386 -0.00006 -0.01047 -0.00554 -0.01601 -1.04987

D11 1.07674 0.00001 -0.01055 -0.00798 -0.01853 1.05821

D12 1.06069 -0.00055 -0.01117 0.00090 -0.01028 1.05042

D13 3.13266 -0.00050 -0.01085 0.00206 -0.00878 3.12388

D14 -1.03992 -0.00042 -0.01093 -0.00037 -0.01130 -1.05122

D15 -0.96800 0.00030 -0.00830 -0.00447 -0.01277 -0.98078

D16 1.10397 0.00035 -0.00798 -0.00330 -0.01128 1.09269

D17 -3.06862 0.00043 -0.00807 -0.00573 -0.01380 -3.08242

D18 2.86048 0.00066 0.16907 0.23828 0.40735 -3.01536

D19 -1.21232 0.00128 0.16857 0.23616 0.40474 -0.80759

D20 0.88738 0.00083 0.16835 0.23923 0.40758 1.29495

D21 1.86716 -0.00088 -0.02771 0.04376 0.01603 1.88319

D22 -1.03009 -0.00145 -0.10299 0.08813 -0.01484 -1.04493

D23 2.72081 -0.00131 -0.19262 -0.02023 -0.21273 2.50808

D24 -0.66734 -0.00090 -0.11697 -0.06408 -0.18117 -0.84851

D25 -3.13938 0.00067 0.12835 -0.00017 0.12818 -3.01120

D26 -1.02278 0.00052 0.12895 -0.00128 0.12768 -0.89510

D27 1.01643 0.00029 0.12913 -0.00214 0.12700 1.14343

D28 -3.12452 0.00020 -0.00560 0.00442 -0.00118 -3.12570

D29 -1.00353 0.00022 -0.00530 0.00572 0.00041 -1.00312

D30 1.03619 0.00027 -0.00517 0.00186 -0.00331 1.03287

D31 1.07724 -0.00010 -0.00691 0.00867 0.00177 1.07901

D32 -3.08495 -0.00008 -0.00661 0.00997 0.00336 -3.08159

D33 -1.04524 -0.00004 -0.00647 0.00611 -0.00036 -1.04560

D34 -1.02369 -0.00022 -0.00817 0.00828 0.00011 -1.02358

D35 1.09730 -0.00020 -0.00787 0.00958 0.00171 1.09901

D36 3.13702 -0.00015 -0.00774 0.00572 -0.00202 3.13500

D37 -3.12620 -0.00007 -0.00138 0.00603 0.00465 -3.12155

D38 -0.99747 -0.00005 -0.00137 0.00717 0.00580 -0.99167

D39 1.02640 -0.00012 -0.00107 0.00428 0.00321 1.02962

D40 1.03061 0.00000 -0.00136 0.00460 0.00325 1.03386

D41 -3.12385 0.00003 -0.00134 0.00575 0.00440 -3.11944

D42 -1.09997 -0.00005 -0.00105 0.00286 0.00181 -1.09816

D43 -0.99960 0.00010 -0.00142 0.00723 0.00581 -0.99379

D44 1.12913 0.00013 -0.00140 0.00837 0.00696 1.13609

D45 -3.13018 0.00006 -0.00111 0.00548 0.00437 -3.12581

D46 3.13774 0.00004 -0.00287 0.00724 0.00438 -3.14107

D47 -1.05058 0.00002 -0.00272 0.00650 0.00378 -1.04680

D48 1.04195 0.00005 -0.00302 0.00806 0.00503 1.04698

D49 1.01265 -0.00005 -0.00289 0.00562 0.00273 1.01538

D50 3.10751 -0.00006 -0.00275 0.00488 0.00213 3.10965

D51 -1.08314 -0.00003 -0.00305 0.00643 0.00338 -1.07976

D52 -1.01760 0.00000 -0.00309 0.00933 0.00624 -1.01136

D53 1.07727 -0.00002 -0.00294 0.00859 0.00565 1.08291

D54 -3.11339 0.00001 -0.00325 0.01014 0.00689 -3.10650

Item Value Threshold Converged?

Maximum Force 0.003355 0.000450 NO

RMS Force 0.000603 0.000300 NO

Maximum Displacement 1.309212 0.001800 NO

RMS Displacement 0.374950 0.001200 NO

Predicted change in Energy=-8.802035D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:30:06 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.067890 -0.491558 -0.239695

2 6 0 -2.862590 0.110243 0.418328

3 8 0 -4.927536 0.129998 -0.807097

4 8 0 -4.072393 -1.838259 -0.185451

5 6 0 -2.349821 -0.621710 1.642596

6 16 0 -1.538507 0.219272 -0.936958

7 6 0 -0.117059 0.725664 -0.037071

8 16 0 1.093074 -0.582755 0.137292

9 16 0 -0.055530 2.195076 0.854012

10 6 0 2.691397 0.316004 0.016764

11 6 0 3.847872 -0.673102 -0.038979

12 6 0 5.202521 0.032917 -0.117474

13 6 0 6.369845 -0.945770 -0.202151

14 1 0 -3.103092 1.144805 0.647898

15 1 0 -4.862167 -2.140058 -0.659816

16 1 0 -1.488348 -0.097011 2.054697

17 1 0 -3.118880 -0.659244 2.418785

18 1 0 -2.051132 -1.641403 1.407062

19 1 0 2.656011 0.929801 -0.883502

20 1 0 2.782652 0.978417 0.874980

21 1 0 3.827070 -1.318429 0.845247

22 1 0 3.729831 -1.331128 -0.905227

23 1 0 5.214848 0.695262 -0.988954

24 1 0 5.326974 0.678753 0.757505

25 1 0 7.327566 -0.423148 -0.256863

26 1 0 6.404757 -1.601769 0.671560

27 1 0 6.292686 -1.582503 -1.087264

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.499302 0.000000

3 O 1.203025 2.401262 0.000000

4 O 1.347801 2.371674 2.234222 0.000000

5 C 2.551807 1.515758 3.634650 2.790879 0.000000

6 S 2.718314 1.897863 3.392691 3.349445 2.831887

7 C 4.139051 2.850275 4.907998 4.715971 3.101923

8 S 5.175517 4.025730 6.135766 5.325646 3.757790

9 S 4.951083 3.523625 5.546195 5.786490 3.717516

10 C 6.812186 5.572285 7.665604 7.101451 5.379268

11 C 7.920387 6.771488 8.845494 8.006850 6.421973

12 C 9.286039 8.083259 10.153968 9.462027 7.782304

13 C 10.447680 9.313324 11.364596 10.480322 8.918559

14 H 2.096745 1.086675 2.544689 3.245411 2.162735

15 H 1.877480 3.197587 2.275767 0.969457 3.730733

16 H 3.474757 2.146905 4.479890 3.837642 1.089620

17 H 2.827764 2.158616 3.781594 3.013521 1.093311

18 H 2.846272 2.168945 4.039067 2.580765 1.088331

19 H 6.902578 5.728996 7.625989 7.308957 5.817793

20 H 7.094593 5.729835 7.937015 7.486643 5.430647

21 H 8.011941 6.853825 9.026146 7.983363 6.266991

22 H 7.870975 6.876726 8.780348 7.851749 6.629996

23 H 9.388245 8.219957 10.159751 9.660083 8.116877

24 H 9.519848 8.216277 10.387690 9.776126 7.836312

25 H 11.395674 10.226420 12.279913 11.487677 9.864036

26 H 10.570681 9.427557 11.558820 10.514803 8.862622

27 H 10.452275 9.431398 11.353613 10.407380 9.114175

6 7 8 9 10

6 S 0.000000

7 C 1.756913 0.000000

8 S 2.953384 1.790750 0.000000

9 S 3.051327 1.719589 3.090198 0.000000

10 C 4.337168 2.838687 1.837643 3.431837 0.000000

11 C 5.533152 4.204430 2.761910 4.925487 1.522784

12 C 6.793213 5.365100 4.163114 5.767653 2.530593

13 C 8.027409 6.700811 5.300124 7.229512 3.894994

14 H 2.411702 3.092128 4.566508 3.230044 5.887389

15 H 4.085335 5.578191 6.206888 6.647467 7.971595

16 H 3.008746 2.633006 3.252096 2.957748 4.668407

17 H 3.811874 4.118268 4.790785 4.469874 6.362400

18 H 3.036334 3.380704 3.552335 4.359686 5.315633

19 H 4.254608 2.906551 2.402627 3.460106 1.090173

20 H 4.746771 3.050254 2.415806 3.088038 1.087958

21 H 5.859198 4.529123 2.918416 5.236352 2.155808

22 H 5.491824 4.447769 2.932473 5.464247 2.154404

23 H 6.770308 5.416294 4.459908 5.781250 2.742829

24 H 7.086407 5.501914 4.461164 5.592844 2.761622

25 H 8.915295 7.535949 6.248978 7.911969 4.702689

26 H 8.306562 6.960833 5.434870 7.495641 4.230326

27 H 8.037199 6.893140 5.434611 7.637964 4.218114

11 12 13 14 15

11 C 0.000000

12 C 1.529608 0.000000

13 C 2.541913 1.525662 0.000000

14 H 7.217513 8.414589 9.738051 0.000000

15 H 8.854500 10.310863 11.304595 3.949024 0.000000

16 H 5.761128 7.035832 8.219790 2.475599 4.788035

17 H 7.387586 8.726822 9.848214 2.528020 3.835315

18 H 6.150357 7.598884 8.601531 3.073419 3.524566

19 H 2.168651 2.806405 4.215990 5.963110 8.123858

20 H 2.167378 2.781133 4.210779 5.892473 8.397842

21 H 1.094867 2.155188 2.775179 7.357555 8.856813

22 H 1.094220 2.156384 2.759074 7.431775 8.633482

23 H 2.154878 1.094683 2.155474 8.489376 10.473471

24 H 2.156303 1.094615 2.155829 8.443651 10.666447

25 H 3.495458 2.177898 1.092409 10.586581 12.316645

26 H 2.811574 2.177188 1.093126 9.896637 11.358076

27 H 2.811232 2.176817 1.093072 9.936279 11.176955

16 17 18 19 20

16 H 0.000000

17 H 1.762754 0.000000

18 H 1.766720 1.768701 0.000000

19 H 5.182959 6.839557 5.832235 0.000000

20 H 4.559574 6.316119 5.523770 1.763706 0.000000

21 H 5.586439 7.152397 5.913815 3.068304 2.523330

22 H 6.124833 7.642338 6.233978 2.503070 3.065988

23 H 7.404346 9.104856 7.999710 2.571726 3.077337

24 H 6.980912 8.711059 7.761540 3.144833 2.564600

25 H 9.119760 10.786245 9.602748 4.903731 4.888936

26 H 8.153433 9.728352 8.487909 4.783321 4.451784

27 H 8.521918 10.085751 8.708871 4.424770 4.767499

21 22 23 24 25

21 H 0.000000

22 H 1.753218 0.000000

23 H 3.056988 2.513672 0.000000

24 H 2.499230 3.058622 1.750133 0.000000

25 H 3.777519 3.766763 2.500076 2.499099 0.000000

26 H 2.599023 3.116847 3.074011 2.523843 1.761446

27 H 3.143818 2.581580 2.521828 3.073931 1.762001

26 27

26 H 0.000000

27 H 1.762496 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 4.52D-01

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.079879 -0.537434 -0.134013

2 6 0 -2.869712 0.208042 0.343133

3 8 0 -4.942170 -0.077547 -0.835602

4 8 0 -4.085883 -1.826371 0.259905

5 6 0 -2.350378 -0.191110 1.710060

6 16 0 -1.553891 -0.033896 -1.002959

7 6 0 -0.126214 0.679980 -0.268884

8 16 0 1.083189 -0.544981 0.224673

9 16 0 -0.057171 2.327106 0.220192

10 6 0 2.681960 0.289243 -0.128785

11 6 0 3.836718 -0.685017 0.061537

12 6 0 5.191817 -0.025875 -0.201024

13 6 0 6.357260 -0.997424 -0.041393

14 1 0 -3.107379 1.267696 0.304267

15 1 0 -4.878986 -2.236287 -0.117988

16 1 0 -1.485658 0.418431 1.970809

17 1 0 -3.114672 -0.028424 2.474729

18 1 0 -2.054543 -1.238060 1.739059

19 1 0 2.641843 0.654860 -1.155037

20 1 0 2.779425 1.147319 0.532925

21 1 0 3.820507 -1.085037 1.080583

22 1 0 3.712424 -1.540807 -0.608904

23 1 0 5.199656 0.393863 -1.212008

24 1 0 5.322561 0.820319 0.480918

25 1 0 7.315336 -0.508512 -0.232214

26 1 0 6.396682 -1.410594 0.969874

27 1 0 6.273759 -1.837517 -0.735711

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2956914 0.1947406 0.1821511

Leave Link 202 at Sat Aug 17 17:30:06 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1105.3211546371 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0553125387 Hartrees.

Nuclear repulsion after empirical dispersion term = 1105.2658420984 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2337

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.35D-10

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 119

GePol: Fraction of low-weight points (<1% of avg) = 5.09%

GePol: Cavity surface area = 307.031 Ang\*\*2

GePol: Cavity volume = 319.417 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0056115779 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1105.2602305205 Hartrees.

Leave Link 301 at Sat Aug 17 17:30:06 2019, MaxMem= 1342177280 cpu: 0.8

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.83D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 296 296 296 296 296 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:30:06 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:30:06 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.993223 0.116118 0.000654 -0.004921 Ang= 13.35 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7554 S= 0.5027

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.63126202243

Leave Link 401 at Sat Aug 17 17:30:07 2019, MaxMem= 1342177280 cpu: 7.5

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16384707.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.22D-15 for 2306.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.82D-15 for 842 412.

Iteration 1 A^-1\*A deviation from unit magnitude is 4.66D-15 for 383.

Iteration 1 A^-1\*A deviation from orthogonality is 6.79D-12 for 1001 995.

E= -1658.43871840375

DIIS: error= 1.59D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.43871840375 IErMin= 1 ErrMin= 1.59D-02

ErrMax= 1.59D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.17D-01 BMatP= 6.17D-01

IDIUse=3 WtCom= 8.41D-01 WtEn= 1.59D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Recover alternate guess density for next cycle.

RMSDP=2.65D-03 MaxDP=9.57D-02 OVMax= 0.00D+00

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.65D-03 CP: 9.90D-01

E= -1658.21795067253 Delta-E= 0.220767731221 Rises=F Damp=F

Switch densities from cycles 1 and 2 for lowest energy.

DIIS: error= 3.19D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 1 EnMin= -1658.43871840375 IErMin= 1 ErrMin= 1.59D-02

ErrMax= 3.19D-02 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.20D+00 BMatP= 6.17D-01

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.797D+00 0.203D+00

Coeff: 0.797D+00 0.203D+00

Gap= 0.118 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=1.38D-02 MaxDP=5.42D-01 DE= 2.21D-01 OVMax= 1.61D-01

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.54D-03 CP: 9.90D-01 2.52D-01

E= -1658.63195136381 Delta-E= -0.414000691285 Rises=F Damp=F

DIIS: error= 1.07D-02 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.63195136381 IErMin= 3 ErrMin= 1.07D-02

ErrMax= 1.07D-02 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.16D-01 BMatP= 6.17D-01

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.303D-01 0.217D+00 0.752D+00

Coeff: 0.303D-01 0.217D+00 0.752D+00

Gap= 0.124 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=6.75D-04 MaxDP=3.55D-02 DE=-4.14D-01 OVMax= 4.91D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 4.20D-04 CP: 9.89D-01 4.09D-01 7.90D-01

E= -1658.66940514453 Delta-E= -0.037453780712 Rises=F Damp=F

DIIS: error= 5.94D-03 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.66940514453 IErMin= 4 ErrMin= 5.94D-03

ErrMax= 5.94D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.56D-02 BMatP= 2.16D-01

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.199D-01 0.884D-01 0.402D+00 0.530D+00

Coeff: -0.199D-01 0.884D-01 0.402D+00 0.530D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=2.42D-04 MaxDP=1.63D-02 DE=-3.75D-02 OVMax= 2.05D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.67D-04 CP: 9.90D-01 4.15D-01 8.15D-01 5.94D-01

E= -1658.67499583104 Delta-E= -0.005590686511 Rises=F Damp=F

DIIS: error= 1.64D-03 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67499583104 IErMin= 5 ErrMin= 1.64D-03

ErrMax= 1.64D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 4.49D-03 BMatP= 3.56D-02

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.888D-02 0.162D-01 0.124D+00 0.301D+00 0.568D+00

Coeff: -0.888D-02 0.162D-01 0.124D+00 0.301D+00 0.568D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.11D-04 MaxDP=5.64D-03 DE=-5.59D-03 OVMax= 8.75D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 7.68D-05 CP: 9.89D-01 4.09D-01 8.26D-01 6.88D-01 6.09D-01

E= -1658.67587892471 Delta-E= -0.000883093673 Rises=F Damp=F

DIIS: error= 1.01D-03 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67587892471 IErMin= 6 ErrMin= 1.01D-03

ErrMax= 1.01D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 6.21D-04 BMatP= 4.49D-03

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.323D-02 0.274D-02 0.455D-01 0.145D+00 0.351D+00 0.459D+00

Coeff: -0.323D-02 0.274D-02 0.455D-01 0.145D+00 0.351D+00 0.459D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.25D-05 MaxDP=1.26D-03 DE=-8.83D-04 OVMax= 3.69D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.20D-05 CP: 9.89D-01 4.06D-01 8.29D-01 7.00D-01 7.03D-01

CP: 8.01D-01

E= -1658.67599553351 Delta-E= -0.000116608804 Rises=F Damp=F

DIIS: error= 2.13D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67599553351 IErMin= 7 ErrMin= 2.13D-04

ErrMax= 2.13D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.46D-05 BMatP= 6.21D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.684D-03-0.511D-03 0.641D-02 0.339D-01 0.104D+00 0.223D+00

Coeff-Com: 0.634D+00

Coeff: -0.684D-03-0.511D-03 0.641D-02 0.339D-01 0.104D+00 0.223D+00

Coeff: 0.634D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.32D-05 MaxDP=4.75D-04 DE=-1.17D-04 OVMax= 1.79D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 9.79D-06 CP: 9.89D-01 4.06D-01 8.29D-01 7.13D-01 7.35D-01

CP: 8.49D-01 9.49D-01

E= -1658.67600343386 Delta-E= -0.000007900343 Rises=F Damp=F

DIIS: error= 5.31D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67600343386 IErMin= 8 ErrMin= 5.31D-05

ErrMax= 5.31D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 5.13D-06 BMatP= 3.46D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.835D-04-0.646D-03-0.263D-02-0.951D-03 0.986D-02 0.525D-01

Coeff-Com: 0.302D+00 0.640D+00

Coeff: 0.835D-04-0.646D-03-0.263D-02-0.951D-03 0.986D-02 0.525D-01

Coeff: 0.302D+00 0.640D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=7.51D-06 MaxDP=2.87D-04 DE=-7.90D-06 OVMax= 1.17D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 3.77D-06 CP: 9.89D-01 4.06D-01 8.29D-01 7.19D-01 7.45D-01

CP: 9.13D-01 1.09D+00 1.06D+00

E= -1658.67600521556 Delta-E= -0.000001781707 Rises=F Damp=F

DIIS: error= 2.29D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67600521556 IErMin= 9 ErrMin= 2.29D-05

ErrMax= 2.29D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 8.00D-07 BMatP= 5.13D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.201D-03-0.141D-03-0.267D-02-0.878D-02-0.206D-01-0.338D-01

Coeff-Com: -0.501D-01 0.211D+00 0.905D+00

Coeff: 0.201D-03-0.141D-03-0.267D-02-0.878D-02-0.206D-01-0.338D-01

Coeff: -0.501D-01 0.211D+00 0.905D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.87D-06 MaxDP=2.00D-04 DE=-1.78D-06 OVMax= 6.94D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.76D-06 CP: 9.89D-01 4.06D-01 8.29D-01 7.22D-01 7.56D-01

CP: 9.46D-01 1.18D+00 1.28D+00 1.03D+00

E= -1658.67600568542 Delta-E= -0.000000469856 Rises=F Damp=F

DIIS: error= 1.14D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67600568542 IErMin=10 ErrMin= 1.14D-05

ErrMax= 1.14D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.49D-07 BMatP= 8.00D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.103D-03 0.603D-04-0.110D-02-0.522D-02-0.145D-01-0.303D-01

Coeff-Com: -0.850D-01 0.352D-02 0.543D+00 0.590D+00

Coeff: 0.103D-03 0.603D-04-0.110D-02-0.522D-02-0.145D-01-0.303D-01

Coeff: -0.850D-01 0.352D-02 0.543D+00 0.590D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.48D-06 MaxDP=1.03D-04 DE=-4.70D-07 OVMax= 4.26D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 8.91D-07 CP: 9.89D-01 4.06D-01 8.29D-01 7.24D-01 7.59D-01

CP: 9.62D-01 1.22D+00 1.38D+00 1.30D+00 8.06D-01

E= -1658.67600579298 Delta-E= -0.000000107561 Rises=F Damp=F

DIIS: error= 4.78D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67600579298 IErMin=11 ErrMin= 4.78D-06

ErrMax= 4.78D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 5.57D-08 BMatP= 3.49D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.354D-04 0.469D-04-0.236D-03-0.167D-02-0.509D-02-0.119D-01

Coeff-Com: -0.392D-01-0.308D-01 0.173D+00 0.333D+00 0.583D+00

Coeff: 0.354D-04 0.469D-04-0.236D-03-0.167D-02-0.509D-02-0.119D-01

Coeff: -0.392D-01-0.308D-01 0.173D+00 0.333D+00 0.583D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.75D-07 MaxDP=4.27D-05 DE=-1.08D-07 OVMax= 1.04D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 3.96D-07 CP: 9.89D-01 4.06D-01 8.29D-01 7.25D-01 7.60D-01

CP: 9.62D-01 1.22D+00 1.40D+00 1.32D+00 9.48D-01

CP: 7.38D-01

E= -1658.67600580958 Delta-E= -0.000000016596 Rises=F Damp=F

DIIS: error= 1.84D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.67600580958 IErMin=12 ErrMin= 1.84D-06

ErrMax= 1.84D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.06D-08 BMatP= 5.57D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.631D-05 0.109D-04 0.146D-03 0.354D-03 0.747D-03 0.712D-03

Coeff-Com: -0.114D-02-0.172D-01-0.353D-01 0.235D-01 0.330D+00 0.698D+00

Coeff: -0.631D-05 0.109D-04 0.146D-03 0.354D-03 0.747D-03 0.712D-03

Coeff: -0.114D-02-0.172D-01-0.353D-01 0.235D-01 0.330D+00 0.698D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.33D-07 MaxDP=1.69D-05 DE=-1.66D-08 OVMax= 3.31D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.58D-07 CP: 9.89D-01 4.06D-01 8.29D-01 7.25D-01 7.60D-01

CP: 9.63D-01 1.22D+00 1.41D+00 1.35D+00 1.01D+00

CP: 9.47D-01 8.78D-01

E= -1658.67600581322 Delta-E= -0.000000003643 Rises=F Damp=F

DIIS: error= 7.04D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1658.67600581322 IErMin=13 ErrMin= 7.04D-07

ErrMax= 7.04D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 8.80D-10 BMatP= 1.06D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.850D-05-0.306D-05 0.995D-04 0.429D-03 0.113D-02 0.221D-02

Coeff-Com: 0.578D-02-0.144D-02-0.395D-01-0.471D-01 0.541D-01 0.277D+00

Coeff-Com: 0.747D+00

Coeff: -0.850D-05-0.306D-05 0.995D-04 0.429D-03 0.113D-02 0.221D-02

Coeff: 0.578D-02-0.144D-02-0.395D-01-0.471D-01 0.541D-01 0.277D+00

Coeff: 0.747D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.09D-07 MaxDP=4.80D-06 DE=-3.64D-09 OVMax= 2.19D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 5.16D-08 CP: 9.89D-01 4.06D-01 8.29D-01 7.25D-01 7.60D-01

CP: 9.63D-01 1.22D+00 1.41D+00 1.36D+00 1.02D+00

CP: 1.01D+00 1.04D+00 9.54D-01

E= -1658.67600581361 Delta-E= -0.000000000389 Rises=F Damp=F

DIIS: error= 1.95D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1658.67600581361 IErMin=14 ErrMin= 1.95D-07

ErrMax= 1.95D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.38D-10 BMatP= 8.80D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.236D-05-0.246D-05 0.167D-04 0.113D-03 0.319D-03 0.764D-03

Coeff-Com: 0.247D-02 0.193D-02-0.110D-01-0.236D-01-0.211D-01 0.108D-01

Coeff-Com: 0.300D+00 0.739D+00

Coeff: -0.236D-05-0.246D-05 0.167D-04 0.113D-03 0.319D-03 0.764D-03

Coeff: 0.247D-02 0.193D-02-0.110D-01-0.236D-01-0.211D-01 0.108D-01

Coeff: 0.300D+00 0.739D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.46D-08 MaxDP=2.87D-06 DE=-3.89D-10 OVMax= 5.40D-06

Cycle 15 Pass 1 IDiag 1:

RMSU= 2.20D-08 CP: 9.89D-01 4.06D-01 8.29D-01 7.25D-01 7.60D-01

CP: 9.63D-01 1.22D+00 1.41D+00 1.36D+00 1.03D+00

CP: 1.03D+00 1.08D+00 1.10D+00 9.00D-01

E= -1658.67600581363 Delta-E= -0.000000000019 Rises=F Damp=F

DIIS: error= 1.03D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1658.67600581363 IErMin=15 ErrMin= 1.03D-07

ErrMax= 1.03D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.66D-11 BMatP= 1.38D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.567D-06-0.449D-06-0.122D-04-0.326D-04-0.799D-04-0.100D-03

Coeff-Com: -0.138D-03 0.958D-03 0.329D-02-0.677D-03-0.173D-01-0.529D-01

Coeff-Com: -0.108D-01 0.348D+00 0.729D+00

Coeff: 0.567D-06-0.449D-06-0.122D-04-0.326D-04-0.799D-04-0.100D-03

Coeff: -0.138D-03 0.958D-03 0.329D-02-0.677D-03-0.173D-01-0.529D-01

Coeff: -0.108D-01 0.348D+00 0.729D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.72D-08 MaxDP=9.54D-07 DE=-1.86D-11 OVMax= 4.02D-06

Cycle 16 Pass 1 IDiag 1:

RMSU= 7.05D-09 CP: 9.89D-01 4.06D-01 8.29D-01 7.25D-01 7.60D-01

CP: 9.63D-01 1.22D+00 1.41D+00 1.36D+00 1.03D+00

CP: 1.04D+00 1.09D+00 1.15D+00 1.08D+00 8.56D-01

E= -1658.67600581369 Delta-E= -0.000000000060 Rises=F Damp=F

DIIS: error= 1.90D-08 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1658.67600581369 IErMin=16 ErrMin= 1.90D-08

ErrMax= 1.90D-08 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.69D-12 BMatP= 2.66D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.362D-06-0.111D-07-0.482D-05-0.175D-04-0.455D-04-0.810D-04

Coeff-Com: -0.220D-03 0.121D-03 0.178D-02 0.147D-02-0.343D-02-0.188D-01

Coeff-Com: -0.253D-01 0.529D-01 0.252D+00 0.740D+00

Coeff: 0.362D-06-0.111D-07-0.482D-05-0.175D-04-0.455D-04-0.810D-04

Coeff: -0.220D-03 0.121D-03 0.178D-02 0.147D-02-0.343D-02-0.188D-01

Coeff: -0.253D-01 0.529D-01 0.252D+00 0.740D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.55D-09 MaxDP=2.18D-07 DE=-6.05D-11 OVMax= 5.00D-07

Error on total polarization charges = 0.04169

SCF Done: E(UB3LYP) = -1658.67600581 A.U. after 16 cycles

NFock= 16 Conv=0.46D-08 -V/T= 2.0020

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655346506602D+03 PE=-6.153387141310D+03 EE= 1.734104398374D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.52

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:30:40 2019, MaxMem= 1342177280 cpu: 384.2

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 336

Leave Link 701 at Sat Aug 17 17:30:41 2019, MaxMem= 1342177280 cpu: 10.2

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:30:41 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:30:44 2019, MaxMem= 1342177280 cpu: 36.2

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.40989857D+00-2.81349529D+00 7.35079763D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.010048934 -0.004558491 0.003735106

2 6 0.000495105 0.002181460 0.001252972

3 8 -0.009304042 0.006859488 -0.005718601

4 8 -0.000120696 -0.002536949 0.001516877

5 6 0.000399848 -0.000788138 0.000761222

6 16 0.000484952 -0.000666222 -0.001163673

7 6 0.000728753 -0.000718764 -0.000088968

8 16 -0.000558604 -0.000729000 -0.000021478

9 16 0.000981604 0.002073056 -0.000365576

10 6 -0.000901731 -0.000730489 -0.000236012

11 6 0.000086437 0.000339227 0.000103551

12 6 0.000082244 -0.000245274 0.000060757

13 6 0.000484185 0.000012375 -0.000034653

14 1 -0.001080319 0.000790014 0.001680671

15 1 -0.001757866 -0.001569747 -0.001154856

16 1 0.000222174 0.000288599 -0.000251905

17 1 -0.001188526 0.000072645 0.000282943

18 1 0.000009253 -0.001397928 -0.000406723

19 1 0.000090381 0.000895347 -0.001212728

20 1 0.000277614 0.000982021 0.001369580

21 1 -0.000002992 -0.000524140 0.001064268

22 1 0.000058659 -0.000509568 -0.001065172

23 1 -0.000002715 0.000535651 -0.001071460

24 1 -0.000030143 0.000462856 0.001050307

25 1 0.001028257 0.000658072 -0.000055304

26 1 -0.000172419 -0.000640225 0.001065657

27 1 -0.000358348 -0.000535876 -0.001096801

-------------------------------------------------------------------

Cartesian Forces: Max 0.010048934 RMS 0.002110083

Leave Link 716 at Sat Aug 17 17:30:44 2019, MaxMem= 1342177280 cpu: 0.3

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.012891269 RMS 0.001603624

Search for a local minimum.

Step number 4 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .16036D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 1 3 4 2

DE= 8.28D-04 DEPred=-8.80D-04 R=-9.41D-01

Trust test=-9.41D-01 RLast= 4.37D-01 DXMaxT set to 7.50D-02

ITU= -1 -1 0 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.83196.

Iteration 1 RMS(Cart)= 0.15302458 RMS(Int)= 0.00622583

Iteration 2 RMS(Cart)= 0.01384693 RMS(Int)= 0.00003238

Iteration 3 RMS(Cart)= 0.00008953 RMS(Int)= 0.00000656

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000656

ITry= 1 IFail=0 DXMaxC= 6.23D-01 DCOld= 1.00D+10 DXMaxT= 7.50D-02 DXLimC= 3.00D+00 Rises=T

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83327 0.00235 -0.00078 0.00000 -0.00078 2.83249

R2 2.27339 0.01289 0.01504 0.00000 0.01504 2.28843

R3 2.54698 0.00412 0.00346 0.00000 0.00346 2.55044

R4 2.86437 0.00099 0.00431 0.00000 0.00431 2.86868

R5 3.58644 0.00282 0.00493 0.00000 0.00493 3.59138

R6 2.05352 0.00135 0.00360 0.00000 0.00360 2.05712

R7 1.83201 0.00249 0.00436 0.00000 0.00436 1.83637

R8 2.05908 0.00022 0.00269 0.00000 0.00269 2.06177

R9 2.06606 0.00103 0.00256 0.00000 0.00256 2.06862

R10 2.05665 0.00140 0.00308 0.00000 0.00308 2.05973

R11 3.32008 0.00157 0.00354 0.00000 0.00354 3.32363

R12 3.38403 0.00008 0.00421 0.00000 0.00421 3.38824

R13 3.24955 0.00162 0.00276 0.00000 0.00276 3.25231

R14 3.47264 0.00090 -0.00123 0.00000 -0.00123 3.47141

R15 2.87765 0.00119 0.00358 0.00000 0.00358 2.88123

R16 2.06013 0.00150 0.00366 0.00000 0.00366 2.06378

R17 2.05594 0.00170 0.00344 0.00000 0.00344 2.05939

R18 2.89054 0.00103 0.00289 0.00000 0.00289 2.89343

R19 2.06900 0.00117 0.00245 0.00000 0.00245 2.07145

R20 2.06778 0.00114 0.00278 0.00000 0.00278 2.07056

R21 2.88308 0.00108 0.00331 0.00000 0.00331 2.88639

R22 2.06865 0.00117 0.00262 0.00000 0.00262 2.07127

R23 2.06852 0.00111 0.00261 0.00000 0.00261 2.07114

R24 2.06435 0.00122 0.00259 0.00000 0.00259 2.06694

R25 2.06571 0.00123 0.00276 0.00000 0.00276 2.06846

R26 2.06561 0.00122 0.00267 0.00000 0.00267 2.06828

A1 2.18226 -0.00109 -0.00104 0.00000 -0.00103 2.18123

A2 1.96718 0.00174 0.00513 0.00000 0.00514 1.97232

A3 2.13274 -0.00061 -0.00350 0.00000 -0.00349 2.12925

A4 2.01818 -0.00075 -0.00193 0.00000 -0.00193 2.01625

A5 1.84472 -0.00119 0.00557 0.00000 0.00557 1.85028

A6 1.87228 0.00016 0.00002 0.00000 0.00002 1.87230

A7 1.94820 0.00139 0.00040 0.00000 0.00041 1.94861

A8 1.94333 -0.00005 -0.00053 0.00000 -0.00053 1.94280

A9 1.82407 0.00049 -0.00349 0.00000 -0.00349 1.82058

A10 1.86929 0.00152 0.00059 0.00000 0.00059 1.86988

A11 1.91814 -0.00027 -0.00381 0.00000 -0.00381 1.91433

A12 1.93054 -0.00082 -0.00262 0.00000 -0.00262 1.92792

A13 1.95033 -0.00006 -0.00057 0.00000 -0.00057 1.94976

A14 1.87986 0.00060 0.00244 0.00000 0.00244 1.88230

A15 1.89235 0.00034 0.00149 0.00000 0.00150 1.89385

A16 1.89076 0.00027 0.00331 0.00000 0.00331 1.89407

A17 1.78774 0.00668 -0.00155 0.00000 -0.00155 1.78619

A18 1.96710 0.00068 -0.00170 0.00000 -0.00166 1.96544

A19 2.14202 0.00030 0.00175 0.00000 0.00179 2.14381

A20 2.15282 -0.00048 0.00638 0.00000 0.00642 2.15925

A21 1.79674 -0.00159 -0.00089 0.00000 -0.00089 1.79585

A22 1.92332 0.00061 -0.00013 0.00000 -0.00013 1.92319

A23 1.87685 -0.00001 0.00336 0.00000 0.00336 1.88021

A24 1.89547 -0.00022 -0.00249 0.00000 -0.00249 1.89298

A25 1.93920 -0.00017 -0.00090 0.00000 -0.00090 1.93830

A26 1.93976 -0.00031 0.00004 0.00000 0.00004 1.93980

A27 1.88740 0.00010 0.00019 0.00000 0.00019 1.88759

A28 1.95482 0.00021 -0.00045 0.00000 -0.00045 1.95437

A29 1.91649 -0.00008 -0.00052 0.00000 -0.00052 1.91598

A30 1.91523 -0.00001 0.00034 0.00000 0.00034 1.91557

A31 1.90744 -0.00013 -0.00033 0.00000 -0.00033 1.90711

A32 1.90973 -0.00015 -0.00162 0.00000 -0.00162 1.90811

A33 1.85756 0.00015 0.00273 0.00000 0.00273 1.86029

A34 1.96532 0.00030 -0.00012 0.00000 -0.00012 1.96520

A35 1.90721 -0.00006 -0.00089 0.00000 -0.00089 1.90632

A36 1.90922 -0.00025 -0.00101 0.00000 -0.00101 1.90821

A37 1.91276 -0.00017 -0.00019 0.00000 -0.00019 1.91257

A38 1.91331 0.00001 -0.00051 0.00000 -0.00051 1.91280

A39 1.85260 0.00017 0.00289 0.00000 0.00289 1.85549

A40 1.94623 0.00003 -0.00177 0.00000 -0.00177 1.94446

A41 1.94447 -0.00026 -0.00229 0.00000 -0.00229 1.94218

A42 1.94401 -0.00042 -0.00197 0.00000 -0.00197 1.94204

A43 1.87458 0.00017 0.00266 0.00000 0.00266 1.87723

A44 1.87550 0.00021 0.00253 0.00000 0.00253 1.87803

A45 1.87538 0.00031 0.00125 0.00000 0.00125 1.87663

D1 2.57743 -0.00037 -0.01549 0.00000 -0.01549 2.56194

D2 -1.54131 0.00001 -0.01197 0.00000 -0.01196 -1.55327

D3 0.39771 0.00011 -0.01344 0.00000 -0.01344 0.38427

D4 -0.61163 0.00044 0.00262 0.00000 0.00262 -0.60901

D5 1.55282 0.00082 0.00614 0.00000 0.00614 1.55896

D6 -2.79136 0.00092 0.00467 0.00000 0.00467 -2.78669

D7 -3.10472 -0.00028 -0.00821 0.00000 -0.00821 -3.11293

D8 -0.00906 0.00049 0.00935 0.00000 0.00935 0.00029

D9 -3.12334 -0.00022 0.00570 0.00000 0.00570 -3.11764

D10 -1.04987 -0.00016 0.00472 0.00000 0.00472 -1.04516

D11 1.05821 -0.00042 0.00674 0.00000 0.00674 1.06495

D12 1.05042 0.00083 -0.00063 0.00000 -0.00063 1.04979

D13 3.12388 0.00090 -0.00161 0.00000 -0.00161 3.12227

D14 -1.05122 0.00063 0.00042 0.00000 0.00042 -1.05081

D15 -0.98078 -0.00063 0.00380 0.00000 0.00380 -0.97697

D16 1.09269 -0.00057 0.00282 0.00000 0.00282 1.09551

D17 -3.08242 -0.00083 0.00485 0.00000 0.00485 -3.07757

D18 -3.01536 -0.00142 -0.19994 0.00000 -0.19994 3.06789

D19 -0.80759 -0.00231 -0.19818 0.00000 -0.19818 -1.00577

D20 1.29495 -0.00132 -0.20073 0.00000 -0.20073 1.09423

D21 1.88319 -0.00034 -0.03611 0.00000 -0.03611 1.84708

D22 -1.04493 -0.00275 -0.07230 0.00000 -0.07230 -1.11723

D23 2.50808 -0.00073 0.01867 0.00000 0.01868 2.52676

D24 -0.84851 0.00181 0.05459 0.00000 0.05458 -0.79393

D25 -3.01120 -0.00009 -0.00115 0.00000 -0.00115 -3.01235

D26 -0.89510 0.00006 -0.00024 0.00000 -0.00024 -0.89534

D27 1.14343 0.00006 0.00047 0.00000 0.00047 1.14390

D28 -3.12570 0.00019 -0.00362 0.00000 -0.00362 -3.12932

D29 -1.00312 0.00011 -0.00470 0.00000 -0.00470 -1.00782

D30 1.03287 0.00024 -0.00149 0.00000 -0.00149 1.03138

D31 1.07901 -0.00009 -0.00715 0.00000 -0.00715 1.07186

D32 -3.08159 -0.00017 -0.00823 0.00000 -0.00823 -3.08982

D33 -1.04560 -0.00004 -0.00502 0.00000 -0.00502 -1.05062

D34 -1.02358 0.00011 -0.00681 0.00000 -0.00681 -1.03038

D35 1.09901 0.00003 -0.00789 0.00000 -0.00789 1.09112

D36 3.13500 0.00017 -0.00468 0.00000 -0.00468 3.13032

D37 -3.12155 0.00004 -0.00500 0.00000 -0.00500 -3.12655

D38 -0.99167 -0.00003 -0.00595 0.00000 -0.00595 -0.99762

D39 1.02962 0.00000 -0.00355 0.00000 -0.00355 1.02606

D40 1.03386 0.00009 -0.00382 0.00000 -0.00382 1.03004

D41 -3.11944 0.00002 -0.00477 0.00000 -0.00477 -3.12421

D42 -1.09816 0.00005 -0.00237 0.00000 -0.00237 -1.10053

D43 -0.99379 0.00006 -0.00600 0.00000 -0.00600 -0.99979

D44 1.13609 -0.00001 -0.00695 0.00000 -0.00695 1.12914

D45 -3.12581 0.00002 -0.00455 0.00000 -0.00455 -3.13036

D46 -3.14107 0.00003 -0.00600 0.00000 -0.00600 3.13612

D47 -1.04680 0.00009 -0.00538 0.00000 -0.00538 -1.05218

D48 1.04698 0.00003 -0.00667 0.00000 -0.00667 1.04031

D49 1.01538 0.00003 -0.00465 0.00000 -0.00465 1.01073

D50 3.10965 0.00009 -0.00403 0.00000 -0.00403 3.10562

D51 -1.07976 0.00003 -0.00532 0.00000 -0.00532 -1.08508

D52 -1.01136 -0.00009 -0.00773 0.00000 -0.00773 -1.01909

D53 1.08291 -0.00003 -0.00712 0.00000 -0.00711 1.07580

D54 -3.10650 -0.00009 -0.00841 0.00000 -0.00841 -3.11490

Item Value Threshold Converged?

Maximum Force 0.012891 0.000450 NO

RMS Force 0.001604 0.000300 NO

Maximum Displacement 0.623247 0.001800 NO

RMS Displacement 0.160699 0.001200 NO

Predicted change in Energy=-5.976182D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:30:44 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.113676 -0.375306 -0.179840

2 6 0 -2.822828 0.038886 0.459557

3 8 0 -4.924030 0.383913 -0.662946

4 8 0 -4.285142 -1.713801 -0.203103

5 6 0 -2.359892 -0.825655 1.618307

6 16 0 -1.536325 0.084914 -0.938510

7 6 0 -0.107645 0.696119 -0.114713

8 16 0 1.120163 -0.578364 0.173306

9 16 0 -0.031439 2.269940 0.577591

10 6 0 2.705818 0.326829 -0.028845

11 6 0 3.876702 -0.649220 0.002917

12 6 0 5.222660 0.065505 -0.145207

13 6 0 6.404858 -0.901613 -0.136339

14 1 0 -2.930458 1.079472 0.760563

15 1 0 -5.127831 -1.886705 -0.655106

16 1 0 -1.429639 -0.426820 2.025656

17 1 0 -3.105566 -0.822746 2.419718

18 1 0 -2.188212 -1.856563 1.308834

19 1 0 2.665250 0.860113 -0.981032

20 1 0 2.786673 1.063831 0.769848

21 1 0 3.866632 -1.210040 0.944701

22 1 0 3.766806 -1.385685 -0.800875

23 1 0 5.225267 0.640317 -1.078457

24 1 0 5.337717 0.794112 0.665413

25 1 0 7.355067 -0.371685 -0.248728

26 1 0 6.449959 -1.465246 0.800890

27 1 0 6.331273 -1.626138 -0.953376

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.498890 0.000000

3 O 1.210983 2.407095 0.000000

4 O 1.349634 2.376846 2.240544 0.000000

5 C 2.551843 1.518039 3.638952 2.795161 0.000000

6 S 2.725825 1.900474 3.412021 3.366333 2.836320

7 C 4.147345 2.852010 4.857530 4.823589 3.223627

8 S 5.249668 4.001265 6.177181 5.536085 3.776237

9 S 4.922976 3.575387 5.388273 5.879938 4.010922

10 C 6.857208 5.557642 7.656365 7.284784 5.450023

11 C 7.997160 6.750238 8.886148 8.233559 6.444821

12 C 9.346800 8.068229 10.164878 9.673034 7.835766

13 C 10.531782 9.294612 11.413746 10.721017 8.938981

14 H 2.097794 1.088580 2.546470 3.250568 2.165821

15 H 1.881147 3.203656 2.279758 0.971765 3.735736

16 H 3.474322 2.147213 4.482927 3.844162 1.091042

17 H 2.823860 2.159764 3.776990 3.010742 1.094668

18 H 2.849154 2.171805 4.048746 2.589102 1.089962

19 H 6.937002 5.733124 7.610855 7.452393 5.903425

20 H 7.112513 5.710805 7.872111 7.659794 5.547718

21 H 8.102264 6.822321 9.077497 8.247585 6.274639

22 H 7.969225 6.858672 8.870239 8.080772 6.610787

23 H 9.436888 8.215780 10.161035 9.836463 8.182680

24 H 9.560900 8.198002 10.355494 9.982153 7.923688

25 H 11.468950 10.210768 12.309294 11.717416 9.903148

26 H 10.664904 9.400187 11.615930 10.784813 8.870779

27 H 10.547980 9.410965 11.437067 10.643255 9.098938

6 7 8 9 10

6 S 0.000000

7 C 1.758789 0.000000

8 S 2.955165 1.792979 0.000000

9 S 3.055746 1.721048 3.098785 0.000000

10 C 4.345318 2.838895 1.836992 3.411161 0.000000

11 C 5.543112 4.206994 2.762709 4.911752 1.524680

12 C 6.805408 5.367565 4.164912 5.743476 2.533046

13 C 8.042331 6.705662 5.303618 7.210711 3.899169

14 H 2.412385 2.980158 4.415974 3.139269 5.740841

15 H 4.106887 5.671444 6.437038 6.691073 8.164435

16 H 3.009905 2.754966 3.155259 3.365170 4.678779

17 H 3.816289 4.209254 4.791960 4.733751 6.410084

18 H 3.040533 3.587677 3.724052 4.713217 5.523416

19 H 4.272700 2.909699 2.406035 3.418925 1.092107

20 H 4.750271 3.048728 2.414523 3.071386 1.089780

21 H 5.866458 4.533286 2.921841 5.238319 2.158066

22 H 5.504980 4.451528 2.933516 5.448892 2.157413

23 H 6.785807 5.419582 4.461387 5.747271 2.747286

24 H 7.094222 5.501833 4.462468 5.568987 2.761745

25 H 8.929789 7.539910 6.252588 7.888057 4.706568

26 H 8.319209 6.965056 5.439407 7.483983 4.233035

27 H 8.051522 6.896079 5.433499 7.616258 4.220516

11 12 13 14 15

11 C 0.000000

12 C 1.531135 0.000000

13 C 2.544536 1.527412 0.000000

14 H 7.063982 8.265705 9.585262 0.000000

15 H 9.112957 10.545320 11.586304 3.953577 0.000000

16 H 5.683150 7.014849 8.141191 2.474234 4.795245

17 H 7.390745 8.759405 9.848239 2.530196 3.830941

18 H 6.320307 7.792920 8.765917 3.077634 3.535439

19 H 2.171142 2.805415 4.219224 5.864573 8.269422

20 H 2.170459 2.787116 4.216089 5.717160 8.565952

21 H 1.096165 2.157250 2.776034 7.174693 9.160657

22 H 1.095691 2.157628 2.763195 7.305371 8.909930

23 H 2.156595 1.096071 2.157909 8.372019 10.665445

24 H 2.157932 1.095998 2.158026 8.273646 10.883853

25 H 3.498481 2.179223 1.093779 10.436309 12.581064

26 H 2.815015 2.178202 1.094584 9.719540 11.676592

27 H 2.809587 2.178030 1.094487 9.799876 11.465947

16 17 18 19 20

16 H 0.000000

17 H 1.766571 0.000000

18 H 1.770150 1.773240 0.000000

19 H 5.240657 6.906477 6.014973 0.000000

20 H 4.645038 6.403103 5.793850 1.766870 0.000000

21 H 5.461903 7.137032 6.100141 3.072019 2.523366

22 H 5.992641 7.610429 6.335207 2.507886 3.070499

23 H 7.420383 9.153173 8.178829 2.571282 3.089068

24 H 7.009853 8.773873 8.004978 3.139621 2.567388

25 H 9.074521 10.805041 9.782895 4.903874 4.895756

26 H 8.041546 9.712954 8.661937 4.786080 4.451613

27 H 8.399092 10.053712 8.817727 4.429665 4.771753

21 22 23 24 25

21 H 0.000000

22 H 1.757228 0.000000

23 H 3.059883 2.511741 0.000000

24 H 2.501743 3.060927 1.754247 0.000000

25 H 3.781044 3.769440 2.499729 2.502886 0.000000

26 H 2.599883 3.125906 3.076559 2.521930 1.765444

27 H 3.138517 2.580225 2.525017 3.076563 1.765881

26 27

26 H 0.000000

27 H 1.765622 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 2.29D-01

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.123032 -0.397477 -0.156445

2 6 0 -2.828889 0.072710 0.435831

3 8 0 -4.934422 0.314398 -0.705407

4 8 0 -4.296414 -1.731930 -0.053086

5 6 0 -2.362155 -0.679911 1.668779

6 16 0 -1.548340 -0.015122 -0.965698

7 6 0 -0.115308 0.668294 -0.208929

8 16 0 1.111995 -0.575631 0.192510

9 16 0 -0.033992 2.300078 0.332062

10 6 0 2.697995 0.303771 -0.100402

11 6 0 3.867678 -0.667026 0.018102

12 6 0 5.213956 0.028250 -0.202126

13 6 0 6.394867 -0.935827 -0.107300

14 1 0 -2.933813 1.137167 0.638141

15 1 0 -5.141270 -1.945070 -0.483338

16 1 0 -1.429621 -0.246190 2.032976

17 1 0 -3.104376 -0.600386 2.469456

18 1 0 -2.193206 -1.735641 1.456863

19 1 0 2.654061 0.745273 -1.098322

20 1 0 2.783279 1.112433 0.625141

21 1 0 3.860891 -1.136832 1.008463

22 1 0 3.753331 -1.475582 -0.712447

23 1 0 5.213336 0.512801 -1.185275

24 1 0 5.333483 0.829614 0.535939

25 1 0 7.345303 -0.420476 -0.272941

26 1 0 6.443228 -1.408958 0.878561

27 1 0 6.316790 -1.733804 -0.852309

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3366765 0.1917069 0.1794556

Leave Link 202 at Sat Aug 17 17:30:44 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1101.0530602327 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0548323733 Hartrees.

Nuclear repulsion after empirical dispersion term = 1100.9982278594 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

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Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2329

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.46D-09

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 98

GePol: Fraction of low-weight points (<1% of avg) = 4.21%

GePol: Cavity surface area = 309.044 Ang\*\*2

GePol: Cavity volume = 319.778 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0056910232 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1100.9925368361 Hartrees.

Leave Link 301 at Sat Aug 17 17:30:44 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:30:44 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:30:44 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Lowest energy guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999932 0.011619 -0.000033 -0.000482 Ang= 1.33 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.998231 -0.059397 0.000056 0.002752 Ang= -6.82 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 1.68D-01

Max alpha theta= 5.581 degrees.

Max beta theta= 5.572 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 17:30:45 2019, MaxMem= 1342177280 cpu: 4.2

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16272723.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.66D-15 for 967.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.45D-15 for 942 144.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.44D-15 for 2299.

Iteration 1 A^-1\*A deviation from orthogonality is 2.58D-11 for 2175 2128.

E= -1658.67679798382

DIIS: error= 3.25D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67679798382 IErMin= 1 ErrMin= 3.25D-04

ErrMax= 3.25D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.72D-05 BMatP= 9.72D-05

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.25D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 88.954 Goal= None Shift= 0.000

Gap= 88.958 Goal= None Shift= 0.000

RMSDP=2.27D-05 MaxDP=1.11D-03 OVMax= 1.38D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.26D-05 CP: 1.00D+00

E= -1658.67680420447 Delta-E= -0.000006220646 Rises=F Damp=F

DIIS: error= 3.43D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67680420447 IErMin= 1 ErrMin= 3.25D-04

ErrMax= 3.43D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.59D-05 BMatP= 9.72D-05

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.43D-03

Coeff-Com: 0.481D+00 0.519D+00

Coeff-En: 0.370D+00 0.630D+00

Coeff: 0.480D+00 0.520D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=1.38D-05 MaxDP=9.43D-04 DE=-6.22D-06 OVMax= 1.28D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.12D-05 CP: 1.00D+00 6.49D-01

E= -1658.67681588512 Delta-E= -0.000011680653 Rises=F Damp=F

DIIS: error= 1.42D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67681588512 IErMin= 3 ErrMin= 1.42D-04

ErrMax= 1.42D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.24D-05 BMatP= 8.59D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.42D-03

Coeff-Com: 0.421D-01 0.335D+00 0.622D+00

Coeff-En: 0.000D+00 0.236D+00 0.764D+00

Coeff: 0.420D-01 0.335D+00 0.623D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=5.83D-06 MaxDP=3.14D-04 DE=-1.17D-05 OVMax= 5.89D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 3.17D-06 CP: 1.00D+00 7.79D-01 6.55D-01

E= -1658.67681930997 Delta-E= -0.000003424851 Rises=F Damp=F

DIIS: error= 7.26D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67681930997 IErMin= 4 ErrMin= 7.26D-05

ErrMax= 7.26D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.92D-06 BMatP= 2.24D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.747D-02 0.182D+00 0.398D+00 0.428D+00

Coeff: -0.747D-02 0.182D+00 0.398D+00 0.428D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=1.95D-06 MaxDP=8.68D-05 DE=-3.42D-06 OVMax= 2.17D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 7.52D-07 CP: 1.00D+00 7.81D-01 7.09D-01 4.67D-01

E= -1658.67681982584 Delta-E= -0.000000515865 Rises=F Damp=F

DIIS: error= 1.05D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67681982584 IErMin= 5 ErrMin= 1.05D-05

ErrMax= 1.05D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.36D-08 BMatP= 2.92D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.640D-02 0.676D-01 0.152D+00 0.218D+00 0.569D+00

Coeff: -0.640D-02 0.676D-01 0.152D+00 0.218D+00 0.569D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=3.89D-07 MaxDP=2.49D-05 DE=-5.16D-07 OVMax= 3.45D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.37D-07 CP: 1.00D+00 7.84D-01 7.07D-01 4.89D-01 7.83D-01

E= -1658.67681984088 Delta-E= -0.000000015043 Rises=F Damp=F

DIIS: error= 1.89D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67681984088 IErMin= 6 ErrMin= 1.89D-06

ErrMax= 1.89D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.13D-09 BMatP= 9.36D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.208D-02 0.163D-01 0.366D-01 0.661D-01 0.265D+00 0.618D+00

Coeff: -0.208D-02 0.163D-01 0.366D-01 0.661D-01 0.265D+00 0.618D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=1.46D-07 MaxDP=6.73D-06 DE=-1.50D-08 OVMax= 1.32D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.08D-07 CP: 1.00D+00 7.85D-01 7.06D-01 5.04D-01 8.76D-01

CP: 8.85D-01

E= -1658.67681984221 Delta-E= -0.000000001324 Rises=F Damp=F

DIIS: error= 5.10D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67681984221 IErMin= 7 ErrMin= 5.10D-07

ErrMax= 5.10D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.83D-10 BMatP= 6.13D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.214D-03 0.306D-03 0.161D-03 0.529D-02 0.461D-01 0.226D+00

Coeff-Com: 0.723D+00

Coeff: -0.214D-03 0.306D-03 0.161D-03 0.529D-02 0.461D-01 0.226D+00

Coeff: 0.723D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=7.00D-08 MaxDP=3.20D-06 DE=-1.32D-09 OVMax= 7.52D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 4.86D-08 CP: 1.00D+00 7.85D-01 7.07D-01 5.06D-01 9.06D-01

CP: 1.01D+00 9.81D-01

E= -1658.67681984231 Delta-E= -0.000000000108 Rises=F Damp=F

DIIS: error= 2.23D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67681984231 IErMin= 8 ErrMin= 2.23D-07

ErrMax= 2.23D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.22D-10 BMatP= 3.83D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.236D-03-0.265D-02-0.645D-02-0.842D-02-0.194D-01 0.203D-01

Coeff-Com: 0.398D+00 0.619D+00

Coeff: 0.236D-03-0.265D-02-0.645D-02-0.842D-02-0.194D-01 0.203D-01

Coeff: 0.398D+00 0.619D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=3.37D-08 MaxDP=1.41D-06 DE=-1.08D-10 OVMax= 4.26D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.80D-08 CP: 1.00D+00 7.85D-01 7.07D-01 5.07D-01 9.25D-01

CP: 1.05D+00 1.14D+00 8.28D-01

E= -1658.67681984235 Delta-E= -0.000000000039 Rises=F Damp=F

DIIS: error= 8.12D-08 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67681984235 IErMin= 9 ErrMin= 8.12D-08

ErrMax= 8.12D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.64D-11 BMatP= 1.22D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.131D-03-0.125D-02-0.295D-02-0.442D-02-0.146D-01-0.216D-01

Coeff-Com: 0.826D-01 0.302D+00 0.660D+00

Coeff: 0.131D-03-0.125D-02-0.295D-02-0.442D-02-0.146D-01-0.216D-01

Coeff: 0.826D-01 0.302D+00 0.660D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=1.87D-08 MaxDP=6.91D-07 DE=-3.91D-11 OVMax= 2.90D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.00D-08 CP: 1.00D+00 7.86D-01 7.07D-01 5.08D-01 9.33D-01

CP: 1.08D+00 1.20D+00 9.91D-01 1.09D+00

E= -1658.67681984235 Delta-E= 0.000000000000 Rises=F Damp=F

DIIS: error= 6.43D-08 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67681984235 IErMin=10 ErrMin= 6.43D-08

ErrMax= 6.43D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.27D-12 BMatP= 1.64D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.151D-04-0.108D-04 0.808D-04-0.274D-03-0.366D-02-0.223D-01

Coeff-Com: -0.755D-01 0.192D-01 0.459D+00 0.623D+00

Coeff: 0.151D-04-0.108D-04 0.808D-04-0.274D-03-0.366D-02-0.223D-01

Coeff: -0.755D-01 0.192D-01 0.459D+00 0.623D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=8.80D-09 MaxDP=3.98D-07 DE=-4.55D-13 OVMax= 9.59D-07

Error on total polarization charges = 0.04175

SCF Done: E(UB3LYP) = -1658.67681984 A.U. after 10 cycles

NFock= 10 Conv=0.88D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655252240363D+03 PE=-6.144749480391D+03 EE= 1.729827883349D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.57

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:31:06 2019, MaxMem= 1342177280 cpu: 246.5

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 345

Leave Link 701 at Sat Aug 17 17:31:07 2019, MaxMem= 1342177280 cpu: 10.2

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:31:07 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:31:10 2019, MaxMem= 1342177280 cpu: 36.0

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.37604246D+00-2.95147839D+00 5.07119569D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000729955 0.000947233 -0.000305697

2 6 0.001299203 0.000870867 0.000616124

3 8 0.000306951 -0.000127590 -0.000219452

4 8 -0.000389209 -0.000835274 -0.000098715

5 6 0.000249668 0.000424191 -0.000166470

6 16 -0.000190396 -0.000027721 -0.000126222

7 6 0.000311226 -0.001069936 -0.000709435

8 16 -0.000889861 0.000474058 0.000033398

9 16 0.000178700 -0.000176076 0.000471803

10 6 0.000209363 -0.000024950 0.000141547

11 6 0.000134240 0.000372462 -0.000102419

12 6 0.000005399 -0.000260999 0.000163166

13 6 -0.000196416 0.000185565 -0.000051439

14 1 -0.000582619 0.000039035 0.000535266

15 1 -0.000270986 -0.000556374 -0.000166663

16 1 0.000077863 0.000009310 -0.000035133

17 1 -0.000164035 -0.000143717 0.000108093

18 1 0.000053997 -0.000280717 0.000020154

19 1 -0.000151685 0.000047849 -0.000195819

20 1 0.000355938 0.000303288 0.000203890

21 1 0.000022639 -0.000183645 0.000177456

22 1 -0.000052724 -0.000093856 -0.000175091

23 1 -0.000032748 0.000168865 -0.000130854

24 1 0.000024209 0.000147004 0.000152272

25 1 0.000303028 0.000008631 0.000012646

26 1 0.000080342 -0.000137986 0.000157149

27 1 0.000037868 -0.000079516 -0.000309555

-------------------------------------------------------------------

Cartesian Forces: Max 0.001299203 RMS 0.000370137

Leave Link 716 at Sat Aug 17 17:31:10 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.001493888 RMS 0.000316120

Search for a local minimum.

Step number 5 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .31612D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 1 3 4 5 2

ITU= 0 -1 -1 0 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.82292.

Iteration 1 RMS(Cart)= 0.02670794 RMS(Int)= 0.00018527

Iteration 2 RMS(Cart)= 0.00033945 RMS(Int)= 0.00000019

Iteration 3 RMS(Cart)= 0.00000004 RMS(Int)= 0.00000019

ITry= 1 IFail=0 DXMaxC= 1.05D-01 DCOld= 1.00D+10 DXMaxT= 7.50D-02 DXLimC= 3.00D+00 Rises=T

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83249 0.00143 -0.00013 0.00000 -0.00013 2.83236

R2 2.28843 -0.00020 0.00250 0.00000 0.00250 2.29093

R3 2.55044 0.00149 0.00058 0.00000 0.00058 2.55101

R4 2.86868 -0.00006 0.00072 0.00000 0.00072 2.86939

R5 3.59138 0.00032 0.00082 0.00000 0.00082 3.59220

R6 2.05712 0.00025 0.00060 0.00000 0.00060 2.05772

R7 1.83637 0.00040 0.00072 0.00000 0.00072 1.83709

R8 2.06177 0.00007 0.00045 0.00000 0.00045 2.06222

R9 2.06862 0.00020 0.00043 0.00000 0.00043 2.06905

R10 2.05973 0.00023 0.00051 0.00000 0.00051 2.06024

R11 3.32363 0.00006 0.00059 0.00000 0.00059 3.32422

R12 3.38824 -0.00065 0.00070 0.00000 0.00070 3.38894

R13 3.25231 0.00002 0.00046 0.00000 0.00046 3.25277

R14 3.47141 0.00080 -0.00020 0.00000 -0.00020 3.47121

R15 2.88123 0.00023 0.00060 0.00000 0.00060 2.88182

R16 2.06378 0.00021 0.00061 0.00000 0.00061 2.06439

R17 2.05939 0.00037 0.00057 0.00000 0.00057 2.05996

R18 2.89343 0.00017 0.00048 0.00000 0.00048 2.89390

R19 2.07145 0.00026 0.00041 0.00000 0.00041 2.07186

R20 2.07056 0.00019 0.00046 0.00000 0.00046 2.07102

R21 2.88639 0.00021 0.00055 0.00000 0.00055 2.88694

R22 2.07127 0.00020 0.00044 0.00000 0.00044 2.07171

R23 2.07114 0.00021 0.00043 0.00000 0.00043 2.07157

R24 2.06694 0.00026 0.00043 0.00000 0.00043 2.06737

R25 2.06846 0.00023 0.00046 0.00000 0.00046 2.06892

R26 2.06828 0.00027 0.00044 0.00000 0.00044 2.06872

A1 2.18123 -0.00013 -0.00018 0.00000 -0.00018 2.18105

A2 1.97232 0.00024 0.00084 0.00000 0.00084 1.97316

A3 2.12925 -0.00011 -0.00059 0.00000 -0.00059 2.12866

A4 2.01625 0.00051 -0.00032 0.00000 -0.00032 2.01593

A5 1.85028 -0.00055 0.00093 0.00000 0.00093 1.85121

A6 1.87230 -0.00006 0.00000 0.00000 0.00000 1.87230

A7 1.94861 -0.00003 0.00007 0.00000 0.00007 1.94867

A8 1.94280 -0.00035 -0.00009 0.00000 -0.00009 1.94272

A9 1.82058 0.00047 -0.00058 0.00000 -0.00058 1.82000

A10 1.86988 0.00094 0.00010 0.00000 0.00010 1.86998

A11 1.91433 -0.00012 -0.00063 0.00000 -0.00063 1.91370

A12 1.92792 0.00001 -0.00044 0.00000 -0.00044 1.92749

A13 1.94976 0.00018 -0.00009 0.00000 -0.00009 1.94967

A14 1.88230 0.00006 0.00040 0.00000 0.00040 1.88271

A15 1.89385 -0.00003 0.00025 0.00000 0.00025 1.89409

A16 1.89407 -0.00011 0.00055 0.00000 0.00055 1.89462

A17 1.78619 0.00042 -0.00026 0.00000 -0.00026 1.78593

A18 1.96544 0.00064 -0.00032 0.00000 -0.00032 1.96512

A19 2.14381 0.00018 0.00026 0.00000 0.00026 2.14407

A20 2.15925 -0.00088 0.00103 0.00000 0.00103 2.16028

A21 1.79585 0.00013 -0.00015 0.00000 -0.00015 1.79570

A22 1.92319 0.00020 -0.00002 0.00000 -0.00002 1.92317

A23 1.88021 -0.00019 0.00056 0.00000 0.00056 1.88077

A24 1.89298 0.00018 -0.00041 0.00000 -0.00041 1.89256

A25 1.93830 -0.00004 -0.00015 0.00000 -0.00015 1.93815

A26 1.93980 -0.00020 0.00001 0.00000 0.00001 1.93981

A27 1.88759 0.00004 0.00003 0.00000 0.00003 1.88762

A28 1.95437 0.00017 -0.00008 0.00000 -0.00008 1.95429

A29 1.91598 0.00004 -0.00009 0.00000 -0.00009 1.91589

A30 1.91557 -0.00015 0.00006 0.00000 0.00006 1.91562

A31 1.90711 -0.00013 -0.00005 0.00000 -0.00005 1.90706

A32 1.90811 0.00003 -0.00027 0.00000 -0.00027 1.90784

A33 1.86029 0.00002 0.00045 0.00000 0.00045 1.86075

A34 1.96520 0.00010 -0.00002 0.00000 -0.00002 1.96518

A35 1.90632 -0.00002 -0.00015 0.00000 -0.00015 1.90617

A36 1.90821 -0.00006 -0.00017 0.00000 -0.00017 1.90805

A37 1.91257 -0.00006 -0.00003 0.00000 -0.00003 1.91254

A38 1.91280 0.00002 -0.00008 0.00000 -0.00008 1.91272

A39 1.85549 0.00000 0.00048 0.00000 0.00048 1.85597

A40 1.94446 0.00019 -0.00029 0.00000 -0.00029 1.94417

A41 1.94218 0.00006 -0.00038 0.00000 -0.00038 1.94180

A42 1.94204 -0.00005 -0.00033 0.00000 -0.00033 1.94171

A43 1.87723 -0.00014 0.00044 0.00000 0.00044 1.87768

A44 1.87803 -0.00010 0.00042 0.00000 0.00042 1.87845

A45 1.87663 0.00001 0.00021 0.00000 0.00021 1.87683

D1 2.56194 0.00020 -0.00258 0.00000 -0.00258 2.55936

D2 -1.55327 0.00009 -0.00199 0.00000 -0.00199 -1.55526

D3 0.38427 0.00035 -0.00223 0.00000 -0.00223 0.38203

D4 -0.60901 0.00006 0.00044 0.00000 0.00044 -0.60858

D5 1.55896 -0.00006 0.00102 0.00000 0.00102 1.55998

D6 -2.78669 0.00020 0.00078 0.00000 0.00078 -2.78591

D7 -3.11293 0.00009 -0.00136 0.00000 -0.00136 -3.11429

D8 0.00029 -0.00005 0.00155 0.00000 0.00155 0.00185

D9 -3.11764 -0.00012 0.00095 0.00000 0.00095 -3.11670

D10 -1.04516 -0.00011 0.00078 0.00000 0.00078 -1.04437

D11 1.06495 -0.00012 0.00112 0.00000 0.00112 1.06607

D12 1.04979 0.00024 -0.00011 0.00000 -0.00011 1.04968

D13 3.12227 0.00026 -0.00027 0.00000 -0.00027 3.12200

D14 -1.05081 0.00025 0.00007 0.00000 0.00007 -1.05074

D15 -0.97697 -0.00010 0.00063 0.00000 0.00063 -0.97634

D16 1.09551 -0.00009 0.00047 0.00000 0.00047 1.09598

D17 -3.07757 -0.00010 0.00081 0.00000 0.00081 -3.07676

D18 3.06789 0.00040 -0.03324 0.00000 -0.03324 3.03465

D19 -1.00577 0.00064 -0.03294 0.00000 -0.03294 -1.03871

D20 1.09423 0.00050 -0.03336 0.00000 -0.03336 1.06086

D21 1.84708 0.00035 -0.00600 0.00000 -0.00600 1.84108

D22 -1.11723 0.00078 -0.01202 0.00000 -0.01202 -1.12925

D23 2.52676 0.00028 0.00310 0.00000 0.00310 2.52986

D24 -0.79393 -0.00003 0.00908 0.00000 0.00908 -0.78485

D25 -3.01235 0.00014 -0.00019 0.00000 -0.00019 -3.01254

D26 -0.89534 0.00010 -0.00004 0.00000 -0.00004 -0.89538

D27 1.14390 0.00015 0.00008 0.00000 0.00008 1.14398

D28 -3.12932 -0.00005 -0.00060 0.00000 -0.00060 -3.12992

D29 -1.00782 -0.00006 -0.00078 0.00000 -0.00078 -1.00860

D30 1.03138 -0.00010 -0.00025 0.00000 -0.00025 1.03113

D31 1.07186 0.00008 -0.00119 0.00000 -0.00119 1.07068

D32 -3.08982 0.00006 -0.00137 0.00000 -0.00137 -3.09118

D33 -1.05062 0.00003 -0.00083 0.00000 -0.00083 -1.05145

D34 -1.03038 0.00018 -0.00113 0.00000 -0.00113 -1.03151

D35 1.09112 0.00017 -0.00131 0.00000 -0.00131 1.08981

D36 3.13032 0.00013 -0.00078 0.00000 -0.00078 3.12954

D37 -3.12655 0.00011 -0.00083 0.00000 -0.00083 -3.12738

D38 -0.99762 0.00010 -0.00099 0.00000 -0.00099 -0.99861

D39 1.02606 0.00006 -0.00059 0.00000 -0.00059 1.02547

D40 1.03004 0.00003 -0.00063 0.00000 -0.00063 1.02941

D41 -3.12421 0.00002 -0.00079 0.00000 -0.00079 -3.12500

D42 -1.10053 -0.00003 -0.00039 0.00000 -0.00039 -1.10092

D43 -0.99979 0.00006 -0.00100 0.00000 -0.00100 -1.00078

D44 1.12914 0.00005 -0.00115 0.00000 -0.00115 1.12799

D45 -3.13036 0.00001 -0.00076 0.00000 -0.00076 -3.13112

D46 3.13612 0.00002 -0.00100 0.00000 -0.00100 3.13512

D47 -1.05218 0.00002 -0.00089 0.00000 -0.00089 -1.05307

D48 1.04031 0.00004 -0.00111 0.00000 -0.00111 1.03920

D49 1.01073 0.00001 -0.00077 0.00000 -0.00077 1.00996

D50 3.10562 0.00001 -0.00067 0.00000 -0.00067 3.10495

D51 -1.08508 0.00003 -0.00088 0.00000 -0.00088 -1.08597

D52 -1.01909 0.00003 -0.00129 0.00000 -0.00129 -1.02038

D53 1.07580 0.00003 -0.00118 0.00000 -0.00118 1.07461

D54 -3.11490 0.00005 -0.00140 0.00000 -0.00140 -3.11630

Item Value Threshold Converged?

Maximum Force 0.001494 0.000450 NO

RMS Force 0.000316 0.000300 NO

Maximum Displacement 0.104988 0.001800 NO

RMS Displacement 0.026795 0.001200 NO

Predicted change in Energy=-8.134179D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:31:10 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.118634 -0.355480 -0.169174

2 6 0 -2.816033 0.026302 0.466389

3 8 0 -4.918207 0.425822 -0.638145

4 8 0 -4.318512 -1.690072 -0.204477

5 6 0 -2.364170 -0.859264 1.614077

6 16 0 -1.535729 0.061707 -0.938253

7 6 0 -0.106298 0.689585 -0.127740

8 16 0 1.124628 -0.578087 0.178744

9 16 0 -0.028421 2.278096 0.530596

10 6 0 2.708012 0.327824 -0.036576

11 6 0 3.881470 -0.645048 0.009539

12 6 0 5.225843 0.070774 -0.149871

13 6 0 6.410697 -0.893286 -0.125638

14 1 0 -2.901019 1.066021 0.778570

15 1 0 -5.168145 -1.840808 -0.652222

16 1 0 -1.423985 -0.482377 2.020153

17 1 0 -3.105887 -0.849548 2.419406

18 1 0 -2.214208 -1.890294 1.292989

19 1 0 2.666707 0.847503 -0.996590

20 1 0 2.786779 1.076532 0.751785

21 1 0 3.873055 -1.191521 0.959986

22 1 0 3.773295 -1.393816 -0.783379

23 1 0 5.226970 0.630671 -1.092416

24 1 0 5.338961 0.812356 0.649489

25 1 0 7.359549 -0.362532 -0.247427

26 1 0 6.457344 -1.441149 0.821101

27 1 0 6.338098 -1.631547 -0.930694

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.498821 0.000000

3 O 1.212305 2.408059 0.000000

4 O 1.349938 2.377697 2.241587 0.000000

5 C 2.551848 1.518418 3.639651 2.795860 0.000000

6 S 2.727072 1.900908 3.415231 3.369130 2.837057

7 C 4.146410 2.852297 4.846086 4.838533 3.245126

8 S 5.259505 3.997104 6.179887 5.568765 3.782982

9 S 4.914798 3.584060 5.357880 5.889955 4.058655

10 C 6.862039 5.555085 7.650536 7.312465 5.464509

11 C 8.007337 6.746553 8.888227 8.269074 6.452011

12 C 9.354214 8.065577 10.161999 9.705580 7.847597

13 C 10.543146 9.291323 11.416951 10.759043 8.945728

14 H 2.097969 1.088897 2.546760 3.251418 2.166334

15 H 1.881757 3.204656 2.280413 0.972149 3.736552

16 H 3.474246 2.147262 4.483409 3.845230 1.091278

17 H 2.823208 2.159954 3.776200 3.010265 1.094894

18 H 2.849633 2.172280 4.050343 2.590480 1.090234

19 H 6.940651 5.733684 7.605079 7.473956 5.919321

20 H 7.112212 5.707534 7.856344 7.684641 5.569841

21 H 8.114250 6.816937 9.080534 8.288926 6.280223

22 H 7.983604 6.855502 8.881126 8.117896 6.610750

23 H 9.442731 8.214928 10.157408 9.863595 8.195756

24 H 9.564525 8.194836 10.344897 10.012901 7.941219

25 H 11.478451 10.207997 12.309242 11.753353 9.912751

26 H 10.677576 9.395465 11.619731 10.827412 8.876176

27 H 10.561794 9.407360 11.446517 10.681486 9.099546

6 7 8 9 10

6 S 0.000000

7 C 1.759101 0.000000

8 S 2.955422 1.793350 0.000000

9 S 3.056448 1.721290 3.100178 0.000000

10 C 4.346629 2.838930 1.836884 3.407831 0.000000

11 C 5.544715 4.207420 2.762842 4.909534 1.524995

12 C 6.807385 5.367974 4.165210 5.739564 2.533453

13 C 8.044753 6.706467 5.304199 7.207672 3.899861

14 H 2.412497 2.962021 4.389615 3.127688 5.715822

15 H 4.110453 5.683332 6.471782 6.691875 8.192426

16 H 3.010096 2.779071 3.145691 3.433160 4.686145

17 H 3.817021 4.225449 4.794947 4.777087 6.420240

18 H 3.041231 3.621813 3.756495 4.768059 5.560220

19 H 4.275670 2.910223 2.406601 3.412127 1.092429

20 H 4.750808 3.048473 2.414309 3.068881 1.090083

21 H 5.867609 4.533977 2.922411 5.238714 2.158441

22 H 5.507112 4.452153 2.933689 5.446331 2.157913

23 H 6.788342 5.420130 4.461631 5.741716 2.748029

24 H 7.095474 5.501818 4.462682 5.565188 2.761765

25 H 8.932143 7.540566 6.253185 7.884182 4.707212

26 H 8.321245 6.965753 5.440162 7.482134 4.233481

27 H 8.053839 6.896566 5.433313 7.612702 4.220913

11 12 13 14 15

11 C 0.000000

12 C 1.531388 0.000000

13 C 2.544972 1.527703 0.000000

14 H 7.037139 8.240049 9.558479 0.000000

15 H 9.152230 10.580241 11.629474 3.954325 0.000000

16 H 5.675992 7.016779 8.133603 2.474003 4.796421

17 H 7.394082 8.767320 9.851118 2.530557 3.830196

18 H 6.352573 7.828282 8.797472 3.078333 3.537236

19 H 2.171556 2.805249 4.219759 5.847950 8.290387

20 H 2.170971 2.788111 4.216969 5.687871 8.588535

21 H 1.096381 2.157592 2.776175 7.142652 9.206741

22 H 1.095935 2.157835 2.763882 7.282647 8.953567

23 H 2.156880 1.096302 2.158313 8.351905 10.693942

24 H 2.158203 1.096228 2.158391 8.244893 10.914806

25 H 3.498982 2.179442 1.094007 10.410220 12.621104

26 H 2.815588 2.178369 1.094826 9.688481 11.725289

27 H 2.809312 2.178231 1.094722 9.775466 11.511514

16 17 18 19 20

16 H 0.000000

17 H 1.767205 0.000000

18 H 1.770720 1.773994 0.000000

19 H 5.253863 6.918949 6.046573 0.000000

20 H 4.665779 6.419834 5.839935 1.767395 0.000000

21 H 5.448437 7.138101 6.136281 3.072634 2.523372

22 H 5.975134 7.607707 6.356728 2.508687 3.071248

23 H 7.427123 9.162993 8.210759 2.571214 3.091019

24 H 7.020861 8.786921 8.047905 3.138750 2.567856

25 H 9.072306 10.810852 9.816504 4.903896 4.896892

26 H 8.029465 9.713906 8.695989 4.786529 4.451580

27 H 8.383198 10.051046 8.840455 4.430479 4.772451

21 22 23 24 25

21 H 0.000000

22 H 1.757895 0.000000

23 H 3.060363 2.511419 0.000000

24 H 2.502161 3.061309 1.754931 0.000000

25 H 3.781627 3.769881 2.499671 2.503517 0.000000

26 H 2.600030 3.127413 3.076980 2.521610 1.766108

27 H 3.137631 2.580005 2.525548 3.076997 1.766526

26 27

26 H 0.000000

27 H 1.766141 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 3.75D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.127798 -0.374363 -0.156114

2 6 0 -2.822315 0.047517 0.447374

3 8 0 -4.928174 0.374681 -0.673816

4 8 0 -4.329473 -1.707990 -0.100450

5 6 0 -2.367194 -0.759190 1.650571

6 16 0 -1.547319 -0.013948 -0.961193

7 6 0 -0.114033 0.665090 -0.200250

8 16 0 1.116468 -0.580834 0.186589

9 16 0 -0.031672 2.294319 0.348995

10 6 0 2.700150 0.306089 -0.095302

11 6 0 3.872561 -0.663207 0.012065

12 6 0 5.217209 0.038195 -0.200317

13 6 0 6.400943 -0.923804 -0.115419

14 1 0 -2.904815 1.106073 0.688928

15 1 0 -5.180990 -1.887347 -0.533836

16 1 0 -1.425002 -0.357150 2.026771

17 1 0 -3.105831 -0.693993 2.456150

18 1 0 -2.219741 -1.809776 1.399301

19 1 0 2.655842 0.759805 -1.088065

20 1 0 2.782848 1.106214 0.640390

21 1 0 3.867079 -1.144227 0.997277

22 1 0 3.760437 -1.463655 -0.728060

23 1 0 5.215449 0.533154 -1.178525

24 1 0 5.334291 0.831901 0.546702

25 1 0 7.349986 -0.403913 -0.276299

26 1 0 6.450508 -1.406544 0.865983

27 1 0 6.324362 -1.714642 -0.868496

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3430641 0.1913131 0.1790532

Leave Link 202 at Sat Aug 17 17:31:10 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1100.4259132937 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0547551906 Hartrees.

Nuclear repulsion after empirical dispersion term = 1100.3711581031 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2327

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.22D-07

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 103

GePol: Fraction of low-weight points (<1% of avg) = 4.43%

GePol: Cavity surface area = 309.487 Ang\*\*2

GePol: Cavity volume = 320.076 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0056836611 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1100.3654744420 Hartrees.

Leave Link 301 at Sat Aug 17 17:31:10 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:31:11 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:31:11 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Lowest energy guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999998 0.002035 -0.000006 -0.000084 Ang= 0.23 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999954 -0.009585 0.000027 0.000398 Ang= -1.10 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 1.77D-01

Max alpha theta= 0.935 degrees.

Max beta theta= 0.934 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 17:31:11 2019, MaxMem= 1342177280 cpu: 4.3

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16244787.

Iteration 1 A\*A^-1 deviation from unit magnitude is 4.55D-15 for 2282.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.33D-15 for 883 765.

Iteration 1 A^-1\*A deviation from unit magnitude is 4.33D-15 for 2297.

Iteration 1 A^-1\*A deviation from orthogonality is 1.33D-11 for 903 899.

E= -1658.67682829527

DIIS: error= 9.57D-06 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67682829527 IErMin= 1 ErrMin= 9.57D-06

ErrMax= 9.57D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.60D-08 BMatP= 8.60D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 88.952 Goal= None Shift= 0.000

Gap= 88.954 Goal= None Shift= 0.000

RMSDP=6.60D-07 MaxDP=3.31D-05 OVMax= 4.05D-05

Cycle 2 Pass 1 IDiag 1:

RMSU= 6.58D-07 CP: 1.00D+00

E= -1658.67682830029 Delta-E= -0.000000005012 Rises=F Damp=F

DIIS: error= 1.04D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67682830029 IErMin= 1 ErrMin= 9.57D-06

ErrMax= 1.04D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.75D-08 BMatP= 8.60D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.484D+00 0.516D+00

Coeff: 0.484D+00 0.516D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=4.08D-07 MaxDP=2.86D-05 DE=-5.01D-09 OVMax= 3.83D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.24D-07 CP: 1.00D+00 6.27D-01

E= -1658.67682831102 Delta-E= -0.000000010731 Rises=F Damp=F

DIIS: error= 4.31D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67682831102 IErMin= 3 ErrMin= 4.31D-06

ErrMax= 4.31D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.93D-08 BMatP= 7.75D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.450D-01 0.330D+00 0.625D+00

Coeff: 0.450D-01 0.330D+00 0.625D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=1.74D-07 MaxDP=9.97D-06 DE=-1.07D-08 OVMax= 1.72D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 9.84D-08 CP: 1.00D+00 7.56D-01 6.46D-01

E= -1658.67682831391 Delta-E= -0.000000002897 Rises=F Damp=F

DIIS: error= 2.18D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67682831391 IErMin= 4 ErrMin= 2.18D-06

ErrMax= 2.18D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.68D-09 BMatP= 1.93D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.730D-02 0.178D+00 0.401D+00 0.429D+00

Coeff: -0.730D-02 0.178D+00 0.401D+00 0.429D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=5.96D-08 MaxDP=2.57D-06 DE=-2.90D-09 OVMax= 6.37D-06

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.27D-08 CP: 1.00D+00 7.57D-01 7.05D-01 4.75D-01

E= -1658.67682831440 Delta-E= -0.000000000483 Rises=F Damp=F

DIIS: error= 3.11D-07 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67682831440 IErMin= 5 ErrMin= 3.11D-07

ErrMax= 3.11D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.45D-11 BMatP= 2.68D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.635D-02 0.670D-01 0.156D+00 0.219D+00 0.565D+00

Coeff: -0.635D-02 0.670D-01 0.156D+00 0.219D+00 0.565D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=1.21D-08 MaxDP=7.55D-07 DE=-4.83D-10 OVMax= 1.06D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.00D-08 CP: 1.00D+00 7.62D-01 7.04D-01 4.90D-01 7.40D-01

E= -1658.67682831439 Delta-E= 0.000000000013 Rises=F Damp=F

DIIS: error= 5.83D-08 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 5 EnMin= -1658.67682831440 IErMin= 6 ErrMin= 5.83D-08

ErrMax= 5.83D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.81D-12 BMatP= 8.45D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.212D-02 0.162D-01 0.377D-01 0.660D-01 0.267D+00 0.615D+00

Coeff: -0.212D-02 0.162D-01 0.377D-01 0.660D-01 0.267D+00 0.615D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=4.38D-09 MaxDP=2.00D-07 DE= 1.27D-11 OVMax= 3.98D-07

Error on total polarization charges = 0.04177

SCF Done: E(UB3LYP) = -1658.67682831 A.U. after 6 cycles

NFock= 6 Conv=0.44D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655237585087D+03 PE=-6.143483189882D+03 EE= 1.729203302039D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.57

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:31:25 2019, MaxMem= 1342177280 cpu: 159.7

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 345

Leave Link 701 at Sat Aug 17 17:31:26 2019, MaxMem= 1342177280 cpu: 10.2

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:31:26 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:31:29 2019, MaxMem= 1342177280 cpu: 36.1

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.37010270D+00-2.96877186D+00 4.67617977D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.002387888 0.001996309 -0.000823755

2 6 0.001409547 0.000604518 0.000567416

3 8 0.001725017 -0.001456872 0.000629632

4 8 -0.000379187 -0.000435129 -0.000356931

5 6 0.000101499 0.000528570 -0.000329514

6 16 -0.000244592 0.000141876 -0.000003515

7 6 0.000283877 -0.001105872 -0.000823471

8 16 -0.000850336 0.000679924 0.000022285

9 16 0.000152920 -0.000434338 0.000559700

10 6 0.000392267 0.000076475 0.000155712

11 6 0.000127270 0.000399002 -0.000105564

12 6 0.000008082 -0.000278634 0.000162383

13 6 -0.000313102 0.000234245 -0.000033090

14 1 -0.000500237 -0.000055529 0.000338829

15 1 -0.000011731 -0.000410840 -0.000055185

16 1 -0.000049567 -0.000145582 0.000031906

17 1 -0.000011031 -0.000167181 0.000059355

18 1 0.000011634 -0.000142064 0.000098325

19 1 -0.000180132 -0.000063614 -0.000002349

20 1 0.000351940 0.000173216 0.000029337

21 1 0.000020607 -0.000145246 0.000027594

22 1 -0.000062559 -0.000018369 -0.000025547

23 1 -0.000020633 0.000119458 0.000017624

24 1 0.000025843 0.000079148 0.000007426

25 1 0.000182964 -0.000097049 0.000034583

26 1 0.000112143 -0.000080743 -0.000003809

27 1 0.000105385 0.000004320 -0.000179375

-------------------------------------------------------------------

Cartesian Forces: Max 0.002387888 RMS 0.000552972

Leave Link 716 at Sat Aug 17 17:31:29 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.002331751 RMS 0.000360203

Search for a local minimum.

Step number 6 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .36020D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 3 4 2 5

6

ITU= 0 0 -1 -1 0 0

Eigenvalues --- 0.00003 0.00291 0.00333 0.00367 0.00400

Eigenvalues --- 0.00486 0.00550 0.00773 0.00997 0.01116

Eigenvalues --- 0.02301 0.02511 0.03514 0.03621 0.04586

Eigenvalues --- 0.04829 0.04855 0.04937 0.05442 0.05465

Eigenvalues --- 0.05539 0.05576 0.05649 0.05839 0.08229

Eigenvalues --- 0.08329 0.08790 0.11245 0.12148 0.12208

Eigenvalues --- 0.13894 0.15848 0.16000 0.16000 0.16000

Eigenvalues --- 0.16026 0.16136 0.16559 0.18549 0.19202

Eigenvalues --- 0.19854 0.21915 0.21917 0.22161 0.23339

Eigenvalues --- 0.24631 0.24948 0.24995 0.25241 0.25324

Eigenvalues --- 0.26618 0.29097 0.29264 0.29428 0.29550

Eigenvalues --- 0.30060 0.30994 0.32478 0.33650 0.33872

Eigenvalues --- 0.33879 0.33898 0.33963 0.34030 0.34040

Eigenvalues --- 0.34098 0.34185 0.34381 0.34497 0.34516

Eigenvalues --- 0.34657 0.39755 0.52602 0.57725 2.51917

Eigenvalue 1 is 2.91D-05 Eigenvector:

D20 D18 D19 D22 D24

1 -0.55496 -0.55379 -0.54789 -0.18797 0.11277

D21 D1 D3 D25 D2

1 -0.10605 -0.04760 -0.04301 -0.03951 -0.03701

En-DIIS/RFO-DIIS IScMMF= 0 using points: 6 5

RFO step: Lambda=-1.53133297D-04.

NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=F DC= 8.47D-06 SmlDif= 1.00D-05

RMS Error= 0.9956195704D-02 NUsed= 2 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: -5.50134 6.50134

Iteration 1 RMS(Cart)= 0.37386958 RMS(Int)= 0.24137214

Iteration 2 RMS(Cart)= 0.30932173 RMS(Int)= 0.19997326

Iteration 3 RMS(Cart)= 0.13689036 RMS(Int)= 0.16719732

Iteration 4 RMS(Cart)= 0.10689455 RMS(Int)= 0.13622420

Iteration 5 RMS(Cart)= 0.10734969 RMS(Int)= 0.10699379

Iteration 6 RMS(Cart)= 0.11046204 RMS(Int)= 0.07881190

Iteration 7 RMS(Cart)= 0.11537871 RMS(Int)= 0.05237021

Iteration 8 RMS(Cart)= 0.10168397 RMS(Int)= 0.03131632

Iteration 9 RMS(Cart)= 0.05931677 RMS(Int)= 0.02270305

Iteration 10 RMS(Cart)= 0.01581192 RMS(Int)= 0.02239194

Iteration 11 RMS(Cart)= 0.00042944 RMS(Int)= 0.02239175

Iteration 12 RMS(Cart)= 0.00003376 RMS(Int)= 0.02239175

Iteration 13 RMS(Cart)= 0.00000646 RMS(Int)= 0.02239175

Iteration 14 RMS(Cart)= 0.00000092 RMS(Int)= 0.02239175

ITry= 1 IFail=0 DXMaxC= 4.11D+00 DCOld= 1.00D+10 DXMaxT= 7.50D-02 DXLimC= 3.00D+00 Rises=F

Iteration 1 RMS(Cart)= 0.36062462 RMS(Int)= 0.22444417

Iteration 2 RMS(Cart)= 0.29309674 RMS(Int)= 0.17875073

Iteration 3 RMS(Cart)= 0.14949786 RMS(Int)= 0.14295704

Iteration 4 RMS(Cart)= 0.11281159 RMS(Int)= 0.11191578

Iteration 5 RMS(Cart)= 0.11394631 RMS(Int)= 0.08298507

Iteration 6 RMS(Cart)= 0.11817100 RMS(Int)= 0.05531322

Iteration 7 RMS(Cart)= 0.11815479 RMS(Int)= 0.03109420

Iteration 8 RMS(Cart)= 0.06451249 RMS(Int)= 0.01917573

Iteration 9 RMS(Cart)= 0.02058635 RMS(Int)= 0.01850934

Iteration 10 RMS(Cart)= 0.00079137 RMS(Int)= 0.01850832

Iteration 11 RMS(Cart)= 0.00009925 RMS(Int)= 0.01850831

Iteration 12 RMS(Cart)= 0.00001326 RMS(Int)= 0.01850831

Iteration 13 RMS(Cart)= 0.00000171 RMS(Int)= 0.01850831

Iteration 14 RMS(Cart)= 0.00000022 RMS(Int)= 0.01850831

ITry= 2 IFail=0 DXMaxC= 4.30D+00 DCOld= 4.11D+00 DXMaxT= 7.50D-02 DXLimC= 3.00D+00 Rises=F

Iteration 1 RMS(Cart)= 0.35154761 RMS(Int)= 0.24639144

Iteration 2 RMS(Cart)= 0.26165408 RMS(Int)= 0.19729865

Iteration 3 RMS(Cart)= 0.14992650 RMS(Int)= 0.15252904

Iteration 4 RMS(Cart)= 0.14890971 RMS(Int)= 0.10988688

Iteration 5 RMS(Cart)= 0.15559357 RMS(Int)= 0.06917182

Iteration 6 RMS(Cart)= 0.16803617 RMS(Int)= 0.03388296

Iteration 7 RMS(Cart)= 0.07203465 RMS(Int)= 0.01673370

Iteration 8 RMS(Cart)= 0.03005304 RMS(Int)= 0.01493894

Iteration 9 RMS(Cart)= 0.00162991 RMS(Int)= 0.01493291

Iteration 10 RMS(Cart)= 0.00018164 RMS(Int)= 0.01493287

Iteration 11 RMS(Cart)= 0.00001894 RMS(Int)= 0.01493287

Iteration 12 RMS(Cart)= 0.00000197 RMS(Int)= 0.01493287

Iteration 13 RMS(Cart)= 0.00000020 RMS(Int)= 0.01493287

ITry= 3 IFail=0 DXMaxC= 4.75D+00 DCOld= 4.11D+00 DXMaxT= 7.50D-02 DXLimC= 3.00D+00 Rises=F

Iteration 1 RMS(Cart)= 0.34025913 RMS(Int)= 0.30061171

Iteration 2 RMS(Cart)= 0.22493692 RMS(Int)= 0.25471050

Iteration 3 RMS(Cart)= 0.15021885 RMS(Int)= 0.21236647

Iteration 4 RMS(Cart)= 0.15111249 RMS(Int)= 0.17218320

Iteration 5 RMS(Cart)= 0.15885450 RMS(Int)= 0.13384764

Iteration 6 RMS(Cart)= 0.13361078 RMS(Int)= 0.09890590

Iteration 7 RMS(Cart)= 0.12047894 RMS(Int)= 0.06774145

Iteration 8 RMS(Cart)= 0.13385812 RMS(Int)= 0.03803701

Iteration 9 RMS(Cart)= 0.13390757 RMS(Int)= 0.01362031

Iteration 10 RMS(Cart)= 0.02252702 RMS(Int)= 0.01169360

Iteration 11 RMS(Cart)= 0.00029316 RMS(Int)= 0.01169286

Iteration 12 RMS(Cart)= 0.00000518 RMS(Int)= 0.01169286

Iteration 13 RMS(Cart)= 0.00000037 RMS(Int)= 0.01169286

ITry= 4 IFail=0 DXMaxC= 5.03D+00 DCOld= 4.11D+00 DXMaxT= 7.50D-02 DXLimC= 3.00D+00 Rises=F

Iteration 1 RMS(Cart)= 0.32837085 RMS(Int)= 0.37331913

Iteration 2 RMS(Cart)= 0.19317662 RMS(Int)= 0.33157744

Iteration 3 RMS(Cart)= 0.15149142 RMS(Int)= 0.29327247

Iteration 4 RMS(Cart)= 0.15393915 RMS(Int)= 0.25716758

Iteration 5 RMS(Cart)= 0.13638129 RMS(Int)= 0.22339482

Iteration 6 RMS(Cart)= 0.11368163 RMS(Int)= 0.19192041

Iteration 7 RMS(Cart)= 0.13090234 RMS(Int)= 0.16130726

Iteration 8 RMS(Cart)= 0.13127090 RMS(Int)= 0.13040274

Iteration 9 RMS(Cart)= 0.13197363 RMS(Int)= 0.09954976

Iteration 10 RMS(Cart)= 0.13294033 RMS(Int)= 0.06881819

Iteration 11 RMS(Cart)= 0.13387738 RMS(Int)= 0.03847622

Iteration 12 RMS(Cart)= 0.13478244 RMS(Int)= 0.01196308

Iteration 13 RMS(Cart)= 0.02815635 RMS(Int)= 0.00881573

Iteration 14 RMS(Cart)= 0.00040870 RMS(Int)= 0.00881301

Iteration 15 RMS(Cart)= 0.00000196 RMS(Int)= 0.00881301

Iteration 16 RMS(Cart)= 0.00000006 RMS(Int)= 0.00881301

ITry= 5 IFail=0 DXMaxC= 5.19D+00 DCOld= 4.11D+00 DXMaxT= 7.50D-02 DXLimC= 3.00D+00 Rises=F

Iteration 1 RMS(Cart)= 0.30854144 RMS(Int)= 0.45520018

Iteration 2 RMS(Cart)= 0.17585019 RMS(Int)= 0.41691636

Iteration 3 RMS(Cart)= 0.15480492 RMS(Int)= 0.38165226

Iteration 4 RMS(Cart)= 0.14251551 RMS(Int)= 0.34829090

Iteration 5 RMS(Cart)= 0.11110870 RMS(Int)= 0.31664486

Iteration 6 RMS(Cart)= 0.12926617 RMS(Int)= 0.28601726

Iteration 7 RMS(Cart)= 0.13025925 RMS(Int)= 0.25505547

Iteration 8 RMS(Cart)= 0.13112182 RMS(Int)= 0.22409149

Iteration 9 RMS(Cart)= 0.13217038 RMS(Int)= 0.19314167

Iteration 10 RMS(Cart)= 0.13318385 RMS(Int)= 0.16220553

Iteration 11 RMS(Cart)= 0.13412956 RMS(Int)= 0.13128992

Iteration 12 RMS(Cart)= 0.13499841 RMS(Int)= 0.10040983

Iteration 13 RMS(Cart)= 0.13579963 RMS(Int)= 0.06960683

Iteration 14 RMS(Cart)= 0.13655812 RMS(Int)= 0.03905698

Iteration 15 RMS(Cart)= 0.13730115 RMS(Int)= 0.01109600

Iteration 16 RMS(Cart)= 0.03338558 RMS(Int)= 0.00632255

Iteration 17 RMS(Cart)= 0.00054705 RMS(Int)= 0.00631471

Iteration 18 RMS(Cart)= 0.00000091 RMS(Int)= 0.00631471

ITry= 6 IFail=0 DXMaxC= 5.15D+00 DCOld= 4.11D+00 DXMaxT= 7.50D-02 DXLimC= 3.00D+00 Rises=F

Iteration 1 RMS(Cart)= 0.33657789 RMS(Int)= 0.39091409

Iteration 2 RMS(Cart)= 0.21943248 RMS(Int)= 0.35362685

Iteration 3 RMS(Cart)= 0.19551058 RMS(Int)= 0.31950078

Iteration 4 RMS(Cart)= 0.18421282 RMS(Int)= 0.28786172

Iteration 5 RMS(Cart)= 0.14294146 RMS(Int)= 0.25670675

Iteration 6 RMS(Cart)= 0.13773312 RMS(Int)= 0.22569283

Iteration 7 RMS(Cart)= 0.13936218 RMS(Int)= 0.19473919

Iteration 8 RMS(Cart)= 0.14049207 RMS(Int)= 0.16378654

Iteration 9 RMS(Cart)= 0.14121417 RMS(Int)= 0.13284533

Iteration 10 RMS(Cart)= 0.14161370 RMS(Int)= 0.10192830

Iteration 11 RMS(Cart)= 0.14171054 RMS(Int)= 0.07106471

Iteration 12 RMS(Cart)= 0.14154970 RMS(Int)= 0.04037284

Iteration 13 RMS(Cart)= 0.14119719 RMS(Int)= 0.01133156

Iteration 14 RMS(Cart)= 0.04095073 RMS(Int)= 0.00424320

Iteration 15 RMS(Cart)= 0.00083998 RMS(Int)= 0.00421554

Iteration 16 RMS(Cart)= 0.00000127 RMS(Int)= 0.00421554

Iteration 17 RMS(Cart)= 0.00000003 RMS(Int)= 0.00421554

ITry= 7 IFail=0 DXMaxC= 6.19D+00 DCOld= 4.11D+00 DXMaxT= 7.50D-02 DXLimC= 3.00D+00 Rises=F

Iteration 1 RMS(Cart)= 0.30389283 RMS(Int)= 0.29288381

Iteration 2 RMS(Cart)= 0.21096022 RMS(Int)= 0.25670098

Iteration 3 RMS(Cart)= 0.18044735 RMS(Int)= 0.22429572

Iteration 4 RMS(Cart)= 0.14977060 RMS(Int)= 0.19310245

Iteration 5 RMS(Cart)= 0.13993756 RMS(Int)= 0.16210376

Iteration 6 RMS(Cart)= 0.14147553 RMS(Int)= 0.13115513

Iteration 7 RMS(Cart)= 0.14270084 RMS(Int)= 0.10022598

Iteration 8 RMS(Cart)= 0.14352010 RMS(Int)= 0.06933777

Iteration 9 RMS(Cart)= 0.14401412 RMS(Int)= 0.03859588

Iteration 10 RMS(Cart)= 0.14420272 RMS(Int)= 0.00952650

Iteration 11 RMS(Cart)= 0.03433047 RMS(Int)= 0.00254938

Iteration 12 RMS(Cart)= 0.00057882 RMS(Int)= 0.00252920

Iteration 13 RMS(Cart)= 0.00000046 RMS(Int)= 0.00252920

ITry= 8 IFail=0 DXMaxC= 5.18D+00 DCOld= 4.11D+00 DXMaxT= 7.50D-02 DXLimC= 3.00D+00 Rises=F

Iteration 1 RMS(Cart)= 0.26998632 RMS(Int)= 0.19531144

Iteration 2 RMS(Cart)= 0.18833993 RMS(Int)= 0.16117731

Iteration 3 RMS(Cart)= 0.15446667 RMS(Int)= 0.12985051

Iteration 4 RMS(Cart)= 0.14346913 RMS(Int)= 0.09887025

Iteration 5 RMS(Cart)= 0.14486613 RMS(Int)= 0.06797801

Iteration 6 RMS(Cart)= 0.14610443 RMS(Int)= 0.03722628

Iteration 7 RMS(Cart)= 0.14697532 RMS(Int)= 0.00833381

Iteration 8 RMS(Cart)= 0.02919196 RMS(Int)= 0.00128367

Iteration 9 RMS(Cart)= 0.00040938 RMS(Int)= 0.00126570

Iteration 10 RMS(Cart)= 0.00000014 RMS(Int)= 0.00126570

ITry= 9 IFail=0 DXMaxC= 3.98D+00 DCOld= 4.11D+00 DXMaxT= 7.50D-02 DXLimC= 3.00D+00 Rises=F

Iteration 1 RMS(Cart)= 0.22436690 RMS(Int)= 0.09868462

Iteration 2 RMS(Cart)= 0.15924253 RMS(Int)= 0.06683764

Iteration 3 RMS(Cart)= 0.14770965 RMS(Int)= 0.03600407

Iteration 4 RMS(Cart)= 0.14922973 RMS(Int)= 0.00753000

Iteration 5 RMS(Cart)= 0.02464136 RMS(Int)= 0.00045431

Iteration 6 RMS(Cart)= 0.00029035 RMS(Int)= 0.00043189

Iteration 7 RMS(Cart)= 0.00000005 RMS(Int)= 0.00043189

ITry=10 IFail=0 DXMaxC= 2.43D+00 DCOld= 3.98D+00 DXMaxT= 7.50D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83236 0.00125 0.00084 0.03391 0.00423 2.83659

R2 2.29093 -0.00233 -0.01625 -0.39743 -0.05599 2.23493

R3 2.55101 0.00096 -0.00374 -0.08311 -0.01205 2.53896

R4 2.86939 -0.00020 -0.00466 -0.11662 -0.01632 2.85307

R5 3.59220 0.00023 -0.00533 -0.12293 -0.01763 3.57457

R6 2.05772 0.00008 -0.00389 -0.09408 -0.01330 2.04442

R7 1.83709 0.00008 -0.00471 -0.11360 -0.01607 1.82102

R8 2.06222 -0.00006 -0.00290 -0.07149 -0.01005 2.05216

R9 2.06905 0.00006 -0.00277 -0.06668 -0.00944 2.05961

R10 2.06024 0.00006 -0.00333 -0.07962 -0.01129 2.04895

R11 3.32422 -0.00002 -0.00383 -0.09515 -0.01335 3.31087

R12 3.38894 -0.00074 -0.00455 -0.12349 -0.01690 3.37204

R13 3.25277 -0.00021 -0.00298 -0.07383 -0.01036 3.24241

R14 3.47121 0.00079 0.00133 0.04486 0.00581 3.47702

R15 2.88182 0.00005 -0.00387 -0.09294 -0.01316 2.86866

R16 2.06439 -0.00001 -0.00395 -0.09501 -0.01345 2.05094

R17 2.05996 0.00015 -0.00372 -0.08709 -0.01243 2.04753

R18 2.89390 0.00005 -0.00312 -0.07469 -0.01059 2.88332

R19 2.07186 0.00011 -0.00265 -0.06226 -0.00888 2.06298

R20 2.07102 0.00003 -0.00300 -0.07200 -0.01020 2.06081

R21 2.88694 0.00005 -0.00357 -0.08526 -0.01210 2.87484

R22 2.07171 0.00005 -0.00283 -0.06775 -0.00961 2.06210

R23 2.07157 0.00005 -0.00282 -0.06730 -0.00955 2.06202

R24 2.06737 0.00010 -0.00280 -0.06634 -0.00943 2.05794

R25 2.06892 0.00007 -0.00298 -0.07085 -0.01006 2.05886

R26 2.06872 0.00010 -0.00289 -0.06827 -0.00972 2.05901

A1 2.18105 -0.00010 0.00117 0.02715 0.00317 2.18422

A2 1.97316 0.00009 -0.00549 -0.13126 -0.01934 1.95382

A3 2.12866 0.00000 0.00383 0.09234 0.01233 2.14099

A4 2.01593 0.00036 0.00209 0.05301 0.00731 2.02325

A5 1.85121 -0.00048 -0.00602 -0.16938 -0.02294 1.82827

A6 1.87230 -0.00007 -0.00002 0.00128 0.00014 1.87244

A7 1.94867 0.00012 -0.00044 -0.01775 -0.00224 1.94643

A8 1.94272 -0.00028 0.00057 0.00797 0.00133 1.94405

A9 1.82000 0.00033 0.00378 0.12710 0.01649 1.83648

A10 1.86998 0.00081 -0.00064 0.00182 -0.00046 1.86952

A11 1.91370 0.00007 0.00412 0.09647 0.01370 1.92740

A12 1.92749 0.00006 0.00283 0.06757 0.00955 1.93703

A13 1.94967 0.00021 0.00061 0.01633 0.00223 1.95190

A14 1.88271 -0.00007 -0.00263 -0.05904 -0.00862 1.87408

A15 1.89409 -0.00012 -0.00161 -0.03840 -0.00549 1.88861

A16 1.89462 -0.00016 -0.00358 -0.08902 -0.01248 1.88215

A17 1.78593 0.00029 0.00168 0.05028 0.00670 1.79264

A18 1.96512 0.00114 0.00205 0.06060 0.00553 1.97066

A19 2.14407 0.00000 -0.00168 -0.03590 -0.00797 2.13610

A20 2.16028 -0.00122 -0.00669 -0.17293 -0.02654 2.13374

A21 1.79570 0.00010 0.00096 0.02226 0.00319 1.79889

A22 1.92317 0.00027 0.00014 0.00433 0.00056 1.92373

A23 1.88077 -0.00028 -0.00363 -0.09605 -0.01323 1.86754

A24 1.89256 0.00022 0.00269 0.07852 0.01054 1.90310

A25 1.93815 0.00004 0.00098 0.01923 0.00288 1.94103

A26 1.93981 -0.00029 -0.00004 -0.00257 -0.00032 1.93949

A27 1.88762 0.00004 -0.00021 -0.00491 -0.00068 1.88694

A28 1.95429 0.00010 0.00049 0.01631 0.00211 1.95640

A29 1.91589 0.00004 0.00056 0.01869 0.00242 1.91831

A30 1.91562 -0.00010 -0.00036 -0.01687 -0.00207 1.91356

A31 1.90706 -0.00009 0.00036 0.00667 0.00102 1.90808

A32 1.90784 0.00006 0.00175 0.04417 0.00617 1.91401

A33 1.86075 -0.00002 -0.00295 -0.07311 -0.01026 1.85048

A34 1.96518 0.00010 0.00013 0.00344 0.00047 1.96565

A35 1.90617 -0.00002 0.00096 0.02277 0.00324 1.90941

A36 1.90805 -0.00003 0.00109 0.02696 0.00378 1.91183

A37 1.91254 -0.00003 0.00020 0.00238 0.00044 1.91297

A38 1.91272 0.00000 0.00055 0.01694 0.00223 1.91495

A39 1.85597 -0.00002 -0.00312 -0.07710 -0.01083 1.84514

A40 1.94417 0.00021 0.00191 0.05112 0.00701 1.95117

A41 1.94180 0.00010 0.00248 0.06260 0.00870 1.95050

A42 1.94171 0.00004 0.00213 0.04990 0.00709 1.94880

A43 1.87768 -0.00018 -0.00287 -0.07267 -0.01015 1.86752

A44 1.87845 -0.00015 -0.00273 -0.06947 -0.00969 1.86876

A45 1.87683 -0.00004 -0.00135 -0.03205 -0.00460 1.87224

D1 2.55936 0.00012 0.01675 0.53889 0.07057 2.62993

D2 -1.55526 0.00015 0.01293 0.42060 0.05493 -1.50033

D3 0.38203 0.00029 0.01453 0.48979 0.06346 0.44549

D4 -0.60858 -0.00014 -0.00283 0.03760 0.00098 -0.60759

D5 1.55998 -0.00011 -0.00664 -0.08070 -0.01466 1.54533

D6 -2.78591 0.00002 -0.00505 -0.01151 -0.00613 -2.79204

D7 -3.11429 0.00015 0.00886 0.22517 0.03150 -3.08279

D8 0.00185 -0.00011 -0.01009 -0.26003 -0.03622 -0.03438

D9 -3.11670 -0.00006 -0.00615 -0.14923 -0.02111 -3.13780

D10 -1.04437 -0.00007 -0.00510 -0.12066 -0.01716 -1.06153

D11 1.06607 -0.00009 -0.00729 -0.17623 -0.02494 1.04113

D12 1.04968 0.00021 0.00068 0.05200 0.00588 1.05556

D13 3.12200 0.00020 0.00174 0.08058 0.00983 3.13183

D14 -1.05074 0.00018 -0.00045 0.02500 0.00205 -1.04869

D15 -0.97634 -0.00010 -0.00411 -0.10026 -0.01414 -0.99048

D16 1.09598 -0.00011 -0.00305 -0.07169 -0.01019 1.08579

D17 -3.07676 -0.00014 -0.00524 -0.12726 -0.01797 -3.09473

D18 3.03465 0.00032 0.21607 6.06310 0.82225 -2.42628

D19 -1.03871 0.00051 0.21416 5.99822 0.81403 -0.22468

D20 1.06086 0.00045 0.21691 6.07575 0.82457 1.88543

D21 1.84108 0.00034 0.03903 1.18268 0.15728 1.99836

D22 -1.12925 0.00096 0.07812 2.11636 0.28977 -0.83948

D23 2.52986 0.00026 -0.02013 -0.30044 -0.05094 2.47892

D24 -0.78485 -0.00022 -0.05904 -1.22824 -0.18110 -0.96595

D25 -3.01254 -0.00004 0.00125 0.47729 0.04898 -2.96356

D26 -0.89538 0.00000 0.00026 0.44333 0.04462 -0.85076

D27 1.14398 0.00001 -0.00051 0.42752 0.04221 1.18619

D28 -3.12992 -0.00008 0.00391 0.14562 0.01847 -3.11145

D29 -1.00860 -0.00009 0.00508 0.17796 0.02288 -0.98572

D30 1.03113 -0.00015 0.00161 0.09034 0.01065 1.04178

D31 1.07068 0.00007 0.00772 0.25032 0.03275 1.10343

D32 -3.09118 0.00005 0.00889 0.28267 0.03716 -3.05402

D33 -1.05145 0.00000 0.00542 0.19505 0.02493 -1.02652

D34 -1.03151 0.00018 0.00736 0.24529 0.03188 -0.99963

D35 1.08981 0.00017 0.00852 0.27764 0.03629 1.12610

D36 3.12954 0.00011 0.00506 0.19002 0.02406 -3.12958

D37 -3.12738 0.00005 0.00540 0.22043 0.02744 -3.09994

D38 -0.99861 0.00007 0.00643 0.24189 0.03062 -0.96799

D39 1.02547 0.00001 0.00384 0.17734 0.02157 1.04704

D40 1.02941 0.00000 0.00412 0.18138 0.02226 1.05167

D41 -3.12500 0.00001 0.00515 0.20284 0.02543 -3.09957

D42 -1.10092 -0.00004 0.00256 0.13829 0.01639 -1.08454

D43 -1.00078 0.00004 0.00648 0.24049 0.03054 -0.97025

D44 1.12799 0.00005 0.00751 0.26194 0.03371 1.16170

D45 -3.13112 -0.00001 0.00492 0.19739 0.02466 -3.10645

D46 3.13512 0.00002 0.00648 0.18098 0.02458 -3.12349

D47 -1.05307 0.00000 0.00582 0.16572 0.02238 -1.03069

D48 1.03920 0.00004 0.00721 0.20074 0.02729 1.06649

D49 1.00996 0.00000 0.00502 0.14790 0.01981 1.02977

D50 3.10495 -0.00002 0.00436 0.13264 0.01761 3.12256

D51 -1.08597 0.00002 0.00575 0.16766 0.02253 -1.06344

D52 -1.02038 0.00005 0.00835 0.22983 0.03134 -0.98904

D53 1.07461 0.00003 0.00769 0.21456 0.02914 1.10375

D54 -3.11630 0.00007 0.00908 0.24959 0.03405 -3.08225

Item Value Threshold Converged?

Maximum Force 0.002332 0.000450 NO

RMS Force 0.000360 0.000300 NO

Maximum Displacement 2.429165 0.001800 NO

RMS Displacement 0.665404 0.001200 NO

Predicted change in Energy=-1.604664D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:31:30 2019, MaxMem= 1342177280 cpu: 2.9

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -3.807026 -0.791343 -0.360572

2 6 0 -2.964689 0.273242 0.279982

3 8 0 -4.652518 -0.598478 -1.164728

4 8 0 -3.413774 -2.025410 -0.003381

5 6 0 -2.475599 -0.023755 1.677131

6 16 0 -1.524701 0.534153 -0.918532

7 6 0 -0.152078 0.697998 0.157896

8 16 0 1.024359 -0.633261 -0.008982

9 16 0 -0.175335 1.733335 1.525935

10 6 0 2.644978 0.217911 0.176913

11 6 0 3.777671 -0.725064 -0.186702

12 6 0 5.146071 -0.074565 -0.006827

13 6 0 6.288148 -0.989377 -0.422919

14 1 0 -3.531449 1.194204 0.247857

15 1 0 -3.961537 -2.650050 -0.491632

16 1 0 -1.881260 0.803082 2.054501

17 1 0 -3.311887 -0.162759 2.362098

18 1 0 -1.867275 -0.920705 1.709305

19 1 0 2.626944 1.081713 -0.479914

20 1 0 2.743490 0.571809 1.196244

21 1 0 3.722624 -1.626305 0.426900

22 1 0 3.661662 -1.056297 -1.219222

23 1 0 5.187245 0.849237 -0.586178

24 1 0 5.274210 0.223836 1.034899

25 1 0 7.258598 -0.518807 -0.272100

26 1 0 6.291507 -1.916782 0.148852

27 1 0 6.223783 -1.259200 -1.476597

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.501061 0.000000

3 O 1.182675 2.386598 0.000000

4 O 1.343560 2.359189 2.217960 0.000000

5 C 2.552279 1.509782 3.625665 2.776854 0.000000

6 S 2.697642 1.891581 3.335672 3.310206 2.820095

7 C 3.980653 2.847122 4.866636 4.252249 2.868405

8 S 4.846741 4.100946 5.793435 4.651359 3.932452

9 S 4.808543 3.385966 5.720331 5.191768 2.898523

10 C 6.552545 5.610887 7.464579 6.463241 5.341289

11 C 7.586979 6.831824 8.487675 7.310361 6.562704

12 C 8.988707 8.123278 9.880666 8.779336 7.805648

13 C 10.097309 9.365003 10.972750 9.766098 9.063437

14 H 2.094881 1.081859 2.542814 3.231545 2.154314

15 H 1.869717 3.183509 2.267037 0.963643 3.716043

16 H 3.476111 2.145569 4.472994 3.818880 1.085959

17 H 2.837818 2.155423 3.798110 3.012530 1.089899

18 H 2.839676 2.161664 4.015156 2.558384 1.084257

19 H 6.702131 5.700651 7.502171 6.809667 5.648968

20 H 6.869580 5.788954 7.851413 6.789444 5.274925

21 H 7.616620 6.953418 8.586775 7.160489 6.522975

22 H 7.522552 6.922703 8.326953 7.244256 6.864471

23 H 9.145453 8.218031 9.962506 9.087396 8.037652

24 H 9.243743 8.273560 10.200710 9.034279 7.780314

25 H 11.069334 10.268775 11.944782 10.781539 9.939777

26 H 10.173815 9.512653 11.101130 9.707083 9.098425

27 H 10.103541 9.479556 10.900814 9.779568 9.335501

6 7 8 9 10

6 S 0.000000

7 C 1.752038 0.000000

8 S 2.947515 1.784406 0.000000

9 S 3.038790 1.715807 3.065292 0.000000

10 C 4.322758 2.838022 1.839961 3.474268 0.000000

11 C 5.498759 4.193660 2.760568 4.960152 1.518029

12 C 6.760247 5.356712 4.159405 5.825395 2.524830

13 C 7.975424 6.682896 5.292035 7.279273 3.884589

14 H 2.413125 3.416791 4.915383 3.631480 6.253514

15 H 4.032315 5.113051 5.399958 6.133512 7.233132

16 H 3.006390 2.568700 3.842351 2.013686 4.935037

17 H 3.800297 3.947632 4.964516 3.759295 6.356429

18 H 3.023161 2.822936 3.375897 3.152811 4.899500

19 H 4.210506 2.876978 2.393990 3.507251 1.085311

20 H 4.763523 3.078701 2.420779 3.158699 1.083506

21 H 5.831997 4.526374 2.908051 5.262048 2.150569

22 H 5.433075 4.417988 2.932406 5.480920 2.146263

23 H 6.727552 5.393041 4.456520 5.830945 2.728369

24 H 7.080775 5.517116 4.459320 5.676024 2.765689

25 H 8.869777 7.522209 6.240838 7.972982 4.693597

26 H 8.260720 6.953916 5.423577 7.552468 4.225503

27 H 7.972864 6.866863 5.438723 7.675884 4.209964

11 12 13 14 15

11 C 0.000000

12 C 1.525786 0.000000

13 C 2.535381 1.521300 0.000000

14 H 7.569390 8.773482 10.081788 0.000000

15 H 7.980845 9.477165 10.383573 3.938288 0.000000

16 H 6.275485 7.375819 8.722943 2.477915 4.768068

17 H 7.554760 8.783885 10.029969 2.521818 3.840890

18 H 5.958064 7.269668 8.429829 3.062376 3.495810

19 H 2.162080 2.811901 4.206789 6.202267 7.571939

20 H 2.159618 2.763616 4.198046 6.376650 7.628020

21 H 1.091683 2.149934 2.776650 7.785172 7.806284

22 H 1.090536 2.153408 2.745361 7.678406 7.821930

23 H 2.150559 1.091216 2.149219 8.765286 9.795619

24 H 2.152290 1.091172 2.150626 8.893856 9.792269

25 H 3.488078 2.174970 1.089016 10.937545 11.422863

26 H 2.802171 2.174862 1.089501 10.304295 10.299165

27 H 2.816487 2.173718 1.089580 10.205758 10.326924

16 17 18 19 20

16 H 0.000000

17 H 1.753328 0.000000

18 H 1.758067 1.757136 0.000000

19 H 5.179266 6.700407 5.385198 0.000000

20 H 4.709395 6.210185 4.873395 1.755873 0.000000

21 H 6.320959 7.441190 5.778356 3.058788 2.526322

22 H 6.700636 7.890161 6.258098 2.487630 3.054217

23 H 7.545798 9.052718 7.626807 2.573029 3.037422

24 H 7.250921 8.696664 7.263993 3.168379 2.559621

25 H 9.523522 10.899584 9.347141 4.904801 4.871517

26 H 8.821750 10.010007 8.366176 4.776541 4.458536

27 H 9.078182 10.337639 8.702285 4.405735 4.754905

21 22 23 24 25

21 H 0.000000

22 H 1.743084 0.000000

23 H 3.049549 2.521747 0.000000

24 H 2.490001 3.052886 1.739707 0.000000

25 H 3.770712 3.758176 2.502138 2.489491 0.000000

26 H 2.600163 3.086770 3.067658 2.530261 1.751228

27 H 3.164469 2.582998 2.512521 3.067360 1.752095

26 27

26 H 0.000000

27 H 1.754732 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 7.89D-01

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -3.832845 -0.875474 0.064595

2 6 0 -2.997258 0.366190 -0.050510

3 8 0 -4.678678 -1.199815 -0.695726

4 8 0 -3.432824 -1.657445 1.081285

5 6 0 -2.507776 0.955322 1.250556

6 16 0 -1.557673 -0.124561 -1.175159

7 6 0 -0.187028 0.651180 -0.407568

8 16 0 0.997217 -0.514967 0.241869

9 16 0 -0.217535 2.294898 0.083609

10 6 0 2.612730 0.289808 -0.115782

11 6 0 3.751177 -0.679762 0.145527

12 6 0 5.115637 -0.041691 -0.097657

13 6 0 6.263357 -1.019527 0.104655

14 1 0 -3.569285 1.086958 -0.619454

15 1 0 -3.976519 -2.452728 1.058309

16 1 0 -1.918566 1.848348 1.064433

17 1 0 -3.343892 1.243876 1.887365

18 1 0 -1.894324 0.254163 1.805233

19 1 0 2.590335 0.597962 -1.156185

20 1 0 2.708243 1.178429 0.496765

21 1 0 3.700749 -1.044047 1.173402

22 1 0 3.638049 -1.557993 -0.491011

23 1 0 5.152031 0.360968 -1.111212

24 1 0 5.241077 0.815571 0.565686

25 1 0 7.230937 -0.545811 -0.054521

26 1 0 6.271523 -1.429343 1.114109

27 1 0 6.201537 -1.860477 -0.585394

---------------------------------------------------------------------

Rotational constants (GHZ): 1.1916351 0.2082893 0.1921188

Leave Link 202 at Sat Aug 17 17:31:30 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1121.8441735975 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0564519566 Hartrees.

Nuclear repulsion after empirical dispersion term = 1121.7877216409 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

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Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2290

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.48D-10

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 102

GePol: Fraction of low-weight points (<1% of avg) = 4.45%

GePol: Cavity surface area = 302.056 Ang\*\*2

GePol: Cavity volume = 314.851 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0054450896 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1121.7822765513 Hartrees.

Leave Link 301 at Sat Aug 17 17:31:30 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.80D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 297 297 297 297 297 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:31:30 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:31:30 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.980428 0.196245 0.000853 -0.015746 Ang= 22.71 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7555 S= 0.5028

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.62254303691

Leave Link 401 at Sat Aug 17 17:31:31 2019, MaxMem= 1342177280 cpu: 7.6

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 740000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 15732300.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.55D-15 for 186.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.50D-15 for 841 377.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.22D-15 for 950.

Iteration 1 A^-1\*A deviation from orthogonality is 1.01D-10 for 1065 1061.

Iteration 2 A\*A^-1 deviation from unit magnitude is 8.66D-15 for 186.

Iteration 2 A\*A^-1 deviation from orthogonality is 5.13D-15 for 844 379.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 380.

Iteration 2 A^-1\*A deviation from orthogonality is 4.43D-16 for 1026 186.

E= -1657.69448151315

DIIS: error= 3.86D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1657.69448151315 IErMin= 1 ErrMin= 3.86D-02

ErrMax= 3.86D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.39D+00 BMatP= 2.39D+00

IDIUse=3 WtCom= 6.14D-01 WtEn= 3.86D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Recover alternate guess density for next cycle.

RMSDP=4.18D-03 MaxDP=1.09D-01 OVMax= 0.00D+00

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.12D-03 CP: 9.56D-01

E= -1658.17405288922 Delta-E= -0.479571376070 Rises=F Damp=F

DIIS: error= 3.66D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.17405288922 IErMin= 2 ErrMin= 3.66D-02

ErrMax= 3.66D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.29D+00 BMatP= 2.39D+00

IDIUse=3 WtCom= 6.34D-01 WtEn= 3.66D-01

Coeff-Com: 0.487D+00 0.513D+00

Coeff-En: 0.000D+00 0.100D+01

Coeff: 0.309D+00 0.691D+00

Gap= 0.116 Goal= None Shift= 0.000

Gap= 0.147 Goal= None Shift= 0.000

RMSDP=3.97D-03 MaxDP=1.62D-01 DE=-4.80D-01 OVMax= 1.87D-01

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.46D-03 CP: 9.61D-01 5.30D-01

E= -1658.21430140357 Delta-E= -0.040248514353 Rises=F Damp=F

DIIS: error= 3.25D-02 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.21430140357 IErMin= 3 ErrMin= 3.25D-02

ErrMax= 3.25D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.00D+00 BMatP= 2.29D+00

IDIUse=3 WtCom= 6.75D-01 WtEn= 3.25D-01

Coeff-Com: 0.537D-01 0.453D+00 0.493D+00

Coeff-En: 0.000D+00 0.480D+00 0.520D+00

Coeff: 0.363D-01 0.462D+00 0.502D+00

Gap= 0.134 Goal= None Shift= 0.000

Gap= 0.142 Goal= None Shift= 0.000

RMSDP=2.19D-03 MaxDP=9.88D-02 DE=-4.02D-02 OVMax= 1.10D-01

Cycle 4 Pass 1 IDiag 1:

RMSU= 8.22D-04 CP: 9.58D-01 7.46D-01 4.71D-01

E= -1658.63512237591 Delta-E= -0.420820972342 Rises=F Damp=F

DIIS: error= 8.94D-03 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.63512237591 IErMin= 4 ErrMin= 8.94D-03

ErrMax= 8.94D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.89D-02 BMatP= 2.00D+00

IDIUse=3 WtCom= 9.11D-01 WtEn= 8.94D-02

Coeff-Com: -0.432D-02 0.169D+00 0.242D+00 0.593D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.394D-02 0.154D+00 0.221D+00 0.630D+00

Gap= 0.117 Goal= None Shift= 0.000

Gap= 0.138 Goal= None Shift= 0.000

RMSDP=5.27D-04 MaxDP=2.66D-02 DE=-4.21D-01 OVMax= 5.37D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.85D-04 CP: 9.59D-01 7.45D-01 5.10D-01 5.94D-01

E= -1658.64469753133 Delta-E= -0.009575155416 Rises=F Damp=F

DIIS: error= 5.90D-03 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.64469753133 IErMin= 5 ErrMin= 5.90D-03

ErrMax= 5.90D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.76D-02 BMatP= 8.89D-02

IDIUse=3 WtCom= 9.41D-01 WtEn= 5.90D-02

Coeff-Com: -0.444D-02 0.259D-01 0.637D-01 0.422D+00 0.493D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.331D+00 0.669D+00

Coeff: -0.418D-02 0.244D-01 0.600D-01 0.416D+00 0.504D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.137 Goal= None Shift= 0.000

RMSDP=2.91D-04 MaxDP=1.46D-02 DE=-9.58D-03 OVMax= 2.75D-02

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.70D-04 CP: 9.57D-01 7.42D-01 5.07D-01 7.58D-01 5.05D-01

E= -1658.65199028428 Delta-E= -0.007292752948 Rises=F Damp=F

DIIS: error= 1.58D-03 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.65199028428 IErMin= 6 ErrMin= 1.58D-03

ErrMax= 1.58D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.96D-03 BMatP= 3.76D-02

IDIUse=3 WtCom= 9.84D-01 WtEn= 1.58D-02

Coeff-Com: -0.519D-03 0.219D-02 0.165D-01 0.187D+00 0.285D+00 0.510D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.510D-03 0.216D-02 0.163D-01 0.184D+00 0.280D+00 0.517D+00

Gap= 0.124 Goal= None Shift= 0.000

Gap= 0.138 Goal= None Shift= 0.000

RMSDP=6.70D-05 MaxDP=2.42D-03 DE=-7.29D-03 OVMax= 6.47D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 4.60D-05 CP: 9.57D-01 7.40D-01 5.07D-01 7.78D-01 5.90D-01

CP: 8.18D-01

E= -1658.65238066749 Delta-E= -0.000390383218 Rises=F Damp=F

DIIS: error= 3.55D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.65238066749 IErMin= 7 ErrMin= 3.55D-04

ErrMax= 3.55D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.32D-04 BMatP= 1.96D-03

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.55D-03

Coeff-Com: -0.267D-03-0.164D-02 0.172D-03 0.392D-01 0.753D-01 0.246D+00

Coeff-Com: 0.641D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00

Coeff-En: 0.100D+01

Coeff: -0.266D-03-0.164D-02 0.171D-03 0.391D-01 0.751D-01 0.246D+00

Coeff: 0.642D+00

Gap= 0.125 Goal= None Shift= 0.000

Gap= 0.138 Goal= None Shift= 0.000

RMSDP=2.56D-05 MaxDP=8.41D-04 DE=-3.90D-04 OVMax= 3.31D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.99D-05 CP: 9.57D-01 7.40D-01 5.07D-01 7.91D-01 6.05D-01

CP: 8.75D-01 9.88D-01

E= -1658.65241376757 Delta-E= -0.000033100074 Rises=F Damp=F

DIIS: error= 1.08D-04 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.65241376757 IErMin= 8 ErrMin= 1.08D-04

ErrMax= 1.08D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.44D-05 BMatP= 1.32D-04

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.08D-03

Coeff-Com: 0.495D-04-0.109D-02-0.173D-02-0.913D-04 0.646D-02 0.562D-01

Coeff-Com: 0.263D+00 0.677D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00

Coeff-En: 0.000D+00 0.100D+01

Coeff: 0.494D-04-0.109D-02-0.173D-02-0.912D-04 0.645D-02 0.561D-01

Coeff: 0.263D+00 0.677D+00

Gap= 0.125 Goal= None Shift= 0.000

Gap= 0.138 Goal= None Shift= 0.000

RMSDP=1.54D-05 MaxDP=6.37D-04 DE=-3.31D-05 OVMax= 2.35D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 6.93D-06 CP: 9.57D-01 7.40D-01 5.06D-01 7.97D-01 6.07D-01

CP: 9.38D-01 1.13D+00 1.09D+00

E= -1658.65241974145 Delta-E= -0.000005973882 Rises=F Damp=F

DIIS: error= 4.67D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.65241974145 IErMin= 9 ErrMin= 4.67D-05

ErrMax= 4.67D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.60D-06 BMatP= 1.44D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.730D-04 0.205D-04-0.970D-03-0.128D-01-0.209D-01-0.511D-01

Coeff-Com: -0.885D-01 0.277D+00 0.897D+00

Coeff: 0.730D-04 0.205D-04-0.970D-03-0.128D-01-0.209D-01-0.511D-01

Coeff: -0.885D-01 0.277D+00 0.897D+00

Gap= 0.125 Goal= None Shift= 0.000

Gap= 0.139 Goal= None Shift= 0.000

RMSDP=1.13D-05 MaxDP=4.44D-04 DE=-5.97D-06 OVMax= 1.69D-03

Cycle 10 Pass 1 IDiag 1:

RMSU= 3.55D-06 CP: 9.57D-01 7.40D-01 5.06D-01 8.02D-01 6.14D-01

CP: 9.72D-01 1.24D+00 1.37D+00 1.08D+00

E= -1658.65242193368 Delta-E= -0.000002192234 Rises=F Damp=F

DIIS: error= 2.29D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.65242193368 IErMin=10 ErrMin= 2.29D-05

ErrMax= 2.29D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.60D-07 BMatP= 3.60D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.301D-04 0.184D-03-0.277D-03-0.712D-02-0.124D-01-0.353D-01

Coeff-Com: -0.839D-01 0.452D-01 0.487D+00 0.607D+00

Coeff: 0.301D-04 0.184D-03-0.277D-03-0.712D-02-0.124D-01-0.353D-01

Coeff: -0.839D-01 0.452D-01 0.487D+00 0.607D+00

Gap= 0.125 Goal= None Shift= 0.000

Gap= 0.139 Goal= None Shift= 0.000

RMSDP=4.05D-06 MaxDP=1.81D-04 DE=-2.19D-06 OVMax= 6.59D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.47D-06 CP: 9.57D-01 7.40D-01 5.06D-01 8.03D-01 6.14D-01

CP: 9.83D-01 1.27D+00 1.46D+00 1.30D+00 9.19D-01

E= -1658.65242224863 Delta-E= -0.000000314942 Rises=F Damp=F

DIIS: error= 7.95D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.65242224863 IErMin=11 ErrMin= 7.95D-06

ErrMax= 7.95D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.53D-07 BMatP= 9.60D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.117D-04 0.807D-04 0.184D-04-0.167D-02-0.310D-02-0.105D-01

Coeff-Com: -0.316D-01-0.214D-01 0.119D+00 0.312D+00 0.637D+00

Coeff: 0.117D-04 0.807D-04 0.184D-04-0.167D-02-0.310D-02-0.105D-01

Coeff: -0.316D-01-0.214D-01 0.119D+00 0.312D+00 0.637D+00

Gap= 0.125 Goal= None Shift= 0.000

Gap= 0.139 Goal= None Shift= 0.000

RMSDP=1.15D-06 MaxDP=7.95D-05 DE=-3.15D-07 OVMax= 2.26D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 8.22D-07 CP: 9.57D-01 7.40D-01 5.06D-01 8.04D-01 6.15D-01

CP: 9.84D-01 1.28D+00 1.47D+00 1.33D+00 1.08D+00

CP: 8.67D-01

E= -1658.65242229407 Delta-E= -0.000000045439 Rises=F Damp=F

DIIS: error= 4.84D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.65242229407 IErMin=12 ErrMin= 4.84D-06

ErrMax= 4.84D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.92D-08 BMatP= 1.53D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.436D-05 0.543D-05 0.911D-04 0.804D-03 0.121D-02 0.242D-02

Coeff-Com: 0.156D-02-0.220D-01-0.511D-01 0.209D-01 0.428D+00 0.618D+00

Coeff: -0.436D-05 0.543D-05 0.911D-04 0.804D-03 0.121D-02 0.242D-02

Coeff: 0.156D-02-0.220D-01-0.511D-01 0.209D-01 0.428D+00 0.618D+00

Gap= 0.125 Goal= None Shift= 0.000

Gap= 0.139 Goal= None Shift= 0.000

RMSDP=7.10D-07 MaxDP=3.73D-05 DE=-4.54D-08 OVMax= 6.88D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 3.35D-07 CP: 9.57D-01 7.40D-01 5.06D-01 8.04D-01 6.14D-01

CP: 9.85D-01 1.28D+00 1.49D+00 1.37D+00 1.15D+00

CP: 1.11D+00 8.25D-01

E= -1658.65242231249 Delta-E= -0.000000018425 Rises=F Damp=F

DIIS: error= 1.30D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1658.65242231249 IErMin=13 ErrMin= 1.30D-06

ErrMax= 1.30D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.73D-09 BMatP= 5.92D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.294D-05-0.113D-04 0.342D-04 0.637D-03 0.103D-02 0.298D-02

Coeff-Com: 0.643D-02-0.416D-02-0.431D-01-0.511D-01 0.876D-01 0.253D+00

Coeff-Com: 0.747D+00

Coeff: -0.294D-05-0.113D-04 0.342D-04 0.637D-03 0.103D-02 0.298D-02

Coeff: 0.643D-02-0.416D-02-0.431D-01-0.511D-01 0.876D-01 0.253D+00

Coeff: 0.747D+00

Gap= 0.125 Goal= None Shift= 0.000

Gap= 0.139 Goal= None Shift= 0.000

RMSDP=2.56D-07 MaxDP=1.67D-05 DE=-1.84D-08 OVMax= 5.01D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 1.13D-07 CP: 9.57D-01 7.40D-01 5.06D-01 8.04D-01 6.14D-01

CP: 9.85D-01 1.28D+00 1.49D+00 1.37D+00 1.18D+00

CP: 1.20D+00 9.89D-01 9.51D-01

E= -1658.65242231425 Delta-E= -0.000000001757 Rises=F Damp=F

DIIS: error= 3.05D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1658.65242231425 IErMin=14 ErrMin= 3.05D-07

ErrMax= 3.05D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.01D-10 BMatP= 3.73D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.349D-06-0.292D-05-0.318D-05 0.653D-04 0.102D-03 0.484D-03

Coeff-Com: 0.129D-02 0.161D-02-0.423D-02-0.162D-01-0.302D-01-0.267D-01

Coeff-Com: 0.219D+00 0.854D+00

Coeff: -0.349D-06-0.292D-05-0.318D-05 0.653D-04 0.102D-03 0.484D-03

Coeff: 0.129D-02 0.161D-02-0.423D-02-0.162D-01-0.302D-01-0.267D-01

Coeff: 0.219D+00 0.854D+00

Gap= 0.125 Goal= None Shift= 0.000

Gap= 0.139 Goal= None Shift= 0.000

RMSDP=9.91D-08 MaxDP=4.03D-06 DE=-1.76D-09 OVMax= 2.24D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 4.17D-08 CP: 9.57D-01 7.40D-01 5.06D-01 8.04D-01 6.14D-01

CP: 9.85D-01 1.28D+00 1.49D+00 1.38D+00 1.19D+00

CP: 1.22D+00 1.03D+00 1.11D+00 1.04D+00

E= -1658.65242231442 Delta-E= -0.000000000172 Rises=F Damp=F

DIIS: error= 1.85D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1658.65242231442 IErMin=15 ErrMin= 1.85D-07

ErrMax= 1.85D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.81D-11 BMatP= 4.01D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.192D-06-0.210D-06-0.581D-05-0.435D-04-0.737D-04-0.107D-03

Coeff-Com: -0.161D-03 0.115D-02 0.313D-02-0.174D-02-0.242D-01-0.475D-01

Coeff-Com: 0.193D-01 0.423D+00 0.627D+00

Coeff: 0.192D-06-0.210D-06-0.581D-05-0.435D-04-0.737D-04-0.107D-03

Coeff: -0.161D-03 0.115D-02 0.313D-02-0.174D-02-0.242D-01-0.475D-01

Coeff: 0.193D-01 0.423D+00 0.627D+00

Gap= 0.125 Goal= None Shift= 0.000

Gap= 0.139 Goal= None Shift= 0.000

RMSDP=3.06D-08 MaxDP=1.65D-06 DE=-1.72D-10 OVMax= 4.52D-06

Cycle 16 Pass 1 IDiag 1:

RMSU= 1.47D-08 CP: 9.57D-01 7.40D-01 5.06D-01 8.04D-01 6.14D-01

CP: 9.85D-01 1.28D+00 1.49D+00 1.38D+00 1.19D+00

CP: 1.23D+00 1.04D+00 1.15D+00 1.17D+00 9.21D-01

E= -1658.65242231442 Delta-E= 0.000000000002 Rises=F Damp=F

DIIS: error= 5.01D-08 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=15 EnMin= -1658.65242231442 IErMin=16 ErrMin= 5.01D-08

ErrMax= 5.01D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.37D-12 BMatP= 9.81D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.145D-06 0.173D-06-0.142D-05-0.216D-04-0.358D-04-0.919D-04

Coeff-Com: -0.228D-03 0.136D-03 0.158D-02 0.142D-02-0.320D-02-0.138D-01

Coeff-Com: -0.203D-01 0.376D-01 0.213D+00 0.784D+00

Coeff: 0.145D-06 0.173D-06-0.142D-05-0.216D-04-0.358D-04-0.919D-04

Coeff: -0.228D-03 0.136D-03 0.158D-02 0.142D-02-0.320D-02-0.138D-01

Coeff: -0.203D-01 0.376D-01 0.213D+00 0.784D+00

Gap= 0.125 Goal= None Shift= 0.000

Gap= 0.139 Goal= None Shift= 0.000

RMSDP=1.09D-08 MaxDP=4.77D-07 DE= 1.82D-12 OVMax= 2.23D-06

Cycle 17 Pass 1 IDiag 1:

RMSU= 5.47D-09 CP: 9.57D-01 7.40D-01 5.06D-01 8.04D-01 6.14D-01

CP: 9.85D-01 1.28D+00 1.49D+00 1.38D+00 1.19D+00

CP: 1.23D+00 1.04D+00 1.16D+00 1.22D+00 1.03D+00

CP: 9.87D-01

E= -1658.65242231445 Delta-E= -0.000000000034 Rises=F Damp=F

DIIS: error= 1.88D-08 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=17 EnMin= -1658.65242231445 IErMin=17 ErrMin= 1.88D-08

ErrMax= 1.88D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.27D-12 BMatP= 7.37D-12

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.467D-08 0.107D-06 0.337D-06-0.204D-05-0.299D-05-0.178D-04

Coeff-Com: -0.551D-04-0.102D-03 0.609D-04 0.631D-03 0.270D-02 0.181D-02

Coeff-Com: -0.997D-02-0.523D-01-0.245D-01 0.281D+00 0.801D+00

Coeff: 0.467D-08 0.107D-06 0.337D-06-0.204D-05-0.299D-05-0.178D-04

Coeff: -0.551D-04-0.102D-03 0.609D-04 0.631D-03 0.270D-02 0.181D-02

Coeff: -0.997D-02-0.523D-01-0.245D-01 0.281D+00 0.801D+00

Gap= 0.125 Goal= None Shift= 0.000

Gap= 0.139 Goal= None Shift= 0.000

RMSDP=4.77D-09 MaxDP=3.22D-07 DE=-3.37D-11 OVMax= 6.51D-07

Error on total polarization charges = 0.04172

SCF Done: E(UB3LYP) = -1658.65242231 A.U. after 17 cycles

NFock= 17 Conv=0.48D-08 -V/T= 2.0018

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7553 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655717749186D+03 PE=-6.187047023622D+03 EE= 1.750894575571D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.42

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7553, after 0.7500

Leave Link 502 at Sat Aug 17 17:32:07 2019, MaxMem= 1342177280 cpu: 419.3

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 330

Leave Link 701 at Sat Aug 17 17:32:08 2019, MaxMem= 1342177280 cpu: 10.1

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:32:08 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:32:11 2019, MaxMem= 1342177280 cpu: 37.3

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.46561426D+00-2.11516195D+00 1.00958727D+00

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.039092983 -0.002490603 0.024733358

2 6 -0.002595399 -0.000433736 0.002965123

3 8 -0.037829652 0.008677803 -0.031359120

4 8 0.002013397 -0.005564695 0.007637869

5 6 -0.015102187 -0.008557624 0.005546907

6 16 0.001322588 0.003869686 -0.001936306

7 6 0.002602632 -0.001715067 0.000753376

8 16 0.001391221 -0.004526563 -0.000169547

9 16 0.028539163 0.023832534 -0.005043878

10 6 -0.003620164 -0.002173432 -0.001862394

11 6 -0.000051850 0.000109026 0.000442163

12 6 0.000376447 -0.000322890 -0.000299205

13 6 0.001728543 -0.000398174 -0.000140960

14 1 -0.003137296 0.003831048 0.000909144

15 1 -0.003507053 -0.006047087 -0.003900240

16 1 -0.008993990 -0.006266767 0.001227894

17 1 -0.006438470 -0.002602525 -0.000456032

18 1 0.002706273 -0.003006772 -0.000225094

19 1 0.000415326 0.003959415 -0.002894034

20 1 -0.000089940 0.001210879 0.004749804

21 1 0.000027441 -0.002445235 0.002467067

22 1 0.000131457 -0.000454824 -0.003664397

23 1 0.000069286 0.002632821 -0.002553914

24 1 0.000003931 0.000187289 0.003545115

25 1 0.002919589 0.002245754 0.000722977

26 1 -0.000884440 -0.002961241 0.002321426

27 1 -0.001089836 -0.000589018 -0.003517103

-------------------------------------------------------------------

Cartesian Forces: Max 0.039092983 RMS 0.009284389

Leave Link 716 at Sat Aug 17 17:32:11 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.167103966 RMS 0.019491545

Search for a local minimum.

Step number 7 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .19492D-01 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 1 3 4 5 6

7 2

DE= 2.44D-02 DEPred=-1.60D-03 R=-1.52D+01

Trust test=-1.52D+01 RLast= 1.50D+00 DXMaxT set to 5.00D-02

ITU= -1 0 0 -1 -1 0 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.92575.

Iteration 1 RMS(Cart)= 0.20304459 RMS(Int)= 0.09124003

Iteration 2 RMS(Cart)= 0.17030819 RMS(Int)= 0.05976458

Iteration 3 RMS(Cart)= 0.15644667 RMS(Int)= 0.02878979

Iteration 4 RMS(Cart)= 0.14073391 RMS(Int)= 0.00515018

Iteration 5 RMS(Cart)= 0.00983532 RMS(Int)= 0.00003342

Iteration 6 RMS(Cart)= 0.00004018 RMS(Int)= 0.00003060

Iteration 7 RMS(Cart)= 0.00000000 RMS(Int)= 0.00003060

ITry= 1 IFail=0 DXMaxC= 2.32D+00 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=T

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83659 0.00520 -0.00394 0.00000 -0.00394 2.83265

R2 2.23493 0.04979 0.05233 0.00000 0.05233 2.28727

R3 2.53896 0.01118 0.01127 0.00000 0.01127 2.55023

R4 2.85307 0.00068 0.01525 0.00000 0.01525 2.86833

R5 3.57457 0.03329 0.01648 0.00000 0.01648 3.59105

R6 2.04442 0.00488 0.01243 0.00000 0.01243 2.05685

R7 1.82102 0.00790 0.01502 0.00000 0.01502 1.83605

R8 2.05216 -0.00928 0.00940 0.00000 0.00940 2.06156

R9 2.05961 0.00499 0.00882 0.00000 0.00882 2.06843

R10 2.04895 0.00402 0.01056 0.00000 0.01056 2.05951

R11 3.31087 0.02403 0.01247 0.00000 0.01247 3.32334

R12 3.37204 0.00358 0.01579 0.00000 0.01579 3.38782

R13 3.24241 0.00999 0.00968 0.00000 0.00968 3.25209

R14 3.47702 0.00034 -0.00542 0.00000 -0.00542 3.47160

R15 2.86866 0.00381 0.01231 0.00000 0.01231 2.88096

R16 2.05094 0.00489 0.01257 0.00000 0.01257 2.06351

R17 2.04753 0.00486 0.01162 0.00000 0.01162 2.05915

R18 2.88332 0.00315 0.00990 0.00000 0.00990 2.89321

R19 2.06298 0.00340 0.00830 0.00000 0.00830 2.07128

R20 2.06081 0.00360 0.00954 0.00000 0.00954 2.07035

R21 2.87484 0.00320 0.01131 0.00000 0.01131 2.88615

R22 2.06210 0.00358 0.00898 0.00000 0.00898 2.07108

R23 2.06202 0.00344 0.00893 0.00000 0.00893 2.07095

R24 2.05794 0.00367 0.00882 0.00000 0.00882 2.06676

R25 2.05886 0.00373 0.00941 0.00000 0.00941 2.06827

R26 2.05901 0.00362 0.00908 0.00000 0.00908 2.06809

A1 2.18422 -0.00274 -0.00297 0.00000 -0.00292 2.18130

A2 1.95382 0.00491 0.01807 0.00000 0.01813 1.97194

A3 2.14099 -0.00185 -0.01153 0.00000 -0.01148 2.12951

A4 2.02325 -0.02637 -0.00684 0.00000 -0.00683 2.01642

A5 1.82827 -0.02379 0.02142 0.00000 0.02142 1.84969

A6 1.87244 0.00835 -0.00013 0.00000 -0.00013 1.87231

A7 1.94643 0.05076 0.00209 0.00000 0.00209 1.94852

A8 1.94405 0.00082 -0.00125 0.00000 -0.00125 1.94280

A9 1.83648 -0.01074 -0.01538 0.00000 -0.01538 1.82111

A10 1.86952 0.00217 0.00044 0.00000 0.00044 1.86997

A11 1.92740 0.00570 -0.01281 0.00000 -0.01281 1.91459

A12 1.93703 -0.00736 -0.00892 0.00000 -0.00892 1.92811

A13 1.95190 0.00029 -0.00208 0.00000 -0.00208 1.94982

A14 1.87408 -0.00011 0.00806 0.00000 0.00807 1.88215

A15 1.88861 -0.00036 0.00513 0.00000 0.00513 1.89374

A16 1.88215 0.00189 0.01166 0.00000 0.01166 1.89380

A17 1.79264 0.16710 -0.00626 0.00000 -0.00626 1.78638

A18 1.97066 -0.01698 -0.00518 0.00000 -0.00500 1.96566

A19 2.13610 0.04126 0.00743 0.00000 0.00762 2.14372

A20 2.13374 -0.01145 0.02477 0.00000 0.02495 2.15869

A21 1.79889 -0.00361 -0.00298 0.00000 -0.00298 1.79591

A22 1.92373 0.00090 -0.00052 0.00000 -0.00052 1.92320

A23 1.86754 0.00033 0.01236 0.00000 0.01236 1.87989

A24 1.90310 -0.00097 -0.00984 0.00000 -0.00984 1.89326

A25 1.94103 -0.00032 -0.00270 0.00000 -0.00270 1.93834

A26 1.93949 -0.00015 0.00030 0.00000 0.00030 1.93979

A27 1.88694 0.00019 0.00063 0.00000 0.00063 1.88757

A28 1.95640 0.00066 -0.00197 0.00000 -0.00197 1.95444

A29 1.91831 -0.00032 -0.00226 0.00000 -0.00226 1.91605

A30 1.91356 0.00008 0.00192 0.00000 0.00192 1.91548

A31 1.90808 -0.00037 -0.00095 0.00000 -0.00095 1.90712

A32 1.91401 -0.00055 -0.00577 0.00000 -0.00577 1.90824

A33 1.85048 0.00048 0.00959 0.00000 0.00959 1.86008

A34 1.96565 0.00067 -0.00044 0.00000 -0.00044 1.96521

A35 1.90941 -0.00023 -0.00303 0.00000 -0.00303 1.90638

A36 1.91183 -0.00056 -0.00353 0.00000 -0.00353 1.90829

A37 1.91297 -0.00028 -0.00041 0.00000 -0.00041 1.91256

A38 1.91495 -0.00014 -0.00208 0.00000 -0.00208 1.91287

A39 1.84514 0.00053 0.01012 0.00000 0.01012 1.85526

A40 1.95117 -0.00059 -0.00655 0.00000 -0.00654 1.94463

A41 1.95050 -0.00099 -0.00813 0.00000 -0.00813 1.94237

A42 1.94880 -0.00093 -0.00662 0.00000 -0.00662 1.94218

A43 1.86752 0.00096 0.00949 0.00000 0.00949 1.87701

A44 1.86876 0.00090 0.00906 0.00000 0.00906 1.87782

A45 1.87224 0.00086 0.00430 0.00000 0.00430 1.87654

D1 2.62993 -0.01522 -0.06584 0.00000 -0.06584 2.56409

D2 -1.50033 0.01506 -0.05125 0.00000 -0.05124 -1.55157

D3 0.44549 -0.00403 -0.05919 0.00000 -0.05919 0.38630

D4 -0.60759 -0.01167 -0.00082 0.00000 -0.00083 -0.60842

D5 1.54533 0.01861 0.01377 0.00000 0.01377 1.55910

D6 -2.79204 -0.00048 0.00583 0.00000 0.00582 -2.78622

D7 -3.08279 -0.00116 -0.02944 0.00000 -0.02945 -3.11224

D8 -0.03438 0.00222 0.03384 0.00000 0.03385 -0.00052

D9 -3.13780 0.00259 0.01973 0.00000 0.01973 -3.11807

D10 -1.06153 0.00143 0.01604 0.00000 0.01604 -1.04549

D11 1.04113 -0.00105 0.02331 0.00000 0.02331 1.06444

D12 1.05556 0.01371 -0.00546 0.00000 -0.00546 1.05010

D13 3.13183 0.01254 -0.00916 0.00000 -0.00916 3.12268

D14 -1.04869 0.01007 -0.00189 0.00000 -0.00189 -1.05057

D15 -0.99048 -0.00602 0.01322 0.00000 0.01322 -0.97726

D16 1.08579 -0.00719 0.00953 0.00000 0.00952 1.09532

D17 -3.09473 -0.00966 0.01680 0.00000 0.01680 -3.07793

D18 -2.42628 -0.01244 -0.76783 0.00000 -0.76782 3.08909

D19 -0.22468 -0.03012 -0.76015 0.00000 -0.76016 -0.98483

D20 1.88543 -0.00774 -0.76999 0.00000 -0.77000 1.11543

D21 1.99836 -0.02146 -0.14680 0.00000 -0.14679 1.85157

D22 -0.83948 -0.06272 -0.27065 0.00000 -0.27066 -1.11014

D23 2.47892 -0.02579 0.04777 0.00000 0.04781 2.52674

D24 -0.96595 0.02586 0.16947 0.00000 0.16942 -0.79653

D25 -2.96356 -0.00043 -0.04538 0.00000 -0.04538 -3.00895

D26 -0.85076 -0.00009 -0.04132 0.00000 -0.04132 -0.89208

D27 1.18619 -0.00019 -0.03906 0.00000 -0.03906 1.14713

D28 -3.11145 0.00058 -0.01722 0.00000 -0.01722 -3.12867

D29 -0.98572 0.00034 -0.02133 0.00000 -0.02133 -1.00706

D30 1.04178 0.00078 -0.00991 0.00000 -0.00991 1.03187

D31 1.10343 -0.00021 -0.03056 0.00000 -0.03056 1.07287

D32 -3.05402 -0.00046 -0.03467 0.00000 -0.03467 -3.08870

D33 -1.02652 -0.00001 -0.02325 0.00000 -0.02325 -1.04977

D34 -0.99963 -0.00013 -0.02974 0.00000 -0.02974 -1.02937

D35 1.12610 -0.00037 -0.03386 0.00000 -0.03386 1.09224

D36 -3.12958 0.00007 -0.02243 0.00000 -0.02243 3.13117

D37 -3.09994 -0.00021 -0.02557 0.00000 -0.02557 -3.12551

D38 -0.96799 -0.00028 -0.02854 0.00000 -0.02854 -0.99653

D39 1.04704 -0.00008 -0.02008 0.00000 -0.02008 1.02696

D40 1.05167 0.00001 -0.02073 0.00000 -0.02073 1.03094

D41 -3.09957 -0.00005 -0.02370 0.00000 -0.02370 -3.12327

D42 -1.08454 0.00014 -0.01525 0.00000 -0.01525 -1.09978

D43 -0.97025 -0.00005 -0.02847 0.00000 -0.02847 -0.99871

D44 1.16170 -0.00011 -0.03144 0.00000 -0.03144 1.13026

D45 -3.10645 0.00008 -0.02298 0.00000 -0.02298 -3.12944

D46 -3.12349 0.00008 -0.02295 0.00000 -0.02295 3.13675

D47 -1.03069 0.00022 -0.02090 0.00000 -0.02090 -1.05159

D48 1.06649 -0.00002 -0.02549 0.00000 -0.02549 1.04100

D49 1.02977 0.00012 -0.01849 0.00000 -0.01849 1.01127

D50 3.12256 0.00025 -0.01644 0.00000 -0.01644 3.10612

D51 -1.06344 0.00002 -0.02103 0.00000 -0.02103 -1.08447

D52 -0.98904 -0.00028 -0.02927 0.00000 -0.02927 -1.01831

D53 1.10375 -0.00015 -0.02721 0.00000 -0.02721 1.07654

D54 -3.08225 -0.00038 -0.03180 0.00000 -0.03180 -3.11405

Item Value Threshold Converged?

Maximum Force 0.167104 0.000450 NO

RMS Force 0.019492 0.000300 NO

Maximum Displacement 2.324547 0.001800 NO

RMS Displacement 0.622177 0.001200 NO

Predicted change in Energy=-1.013641D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:32:11 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.109427 -0.388457 -0.198548

2 6 0 -2.828314 0.036619 0.453360

3 8 0 -4.926039 0.364118 -0.679970

4 8 0 -4.261874 -1.728803 -0.236655

5 6 0 -2.360176 -0.833883 1.605293

6 16 0 -1.534875 0.114883 -0.936617

7 6 0 -0.109171 0.702581 -0.091167

8 16 0 1.118099 -0.578966 0.164630

9 16 0 -0.037084 2.254534 0.649004

10 6 0 2.704148 0.332107 -0.006535

11 6 0 3.874906 -0.644387 -0.003427

12 6 0 5.221078 0.074522 -0.126000

13 6 0 6.403061 -0.892473 -0.146921

14 1 0 -2.952247 1.072118 0.764936

15 1 0 -5.098759 -1.908869 -0.696215

16 1 0 -1.437929 -0.427015 2.022484

17 1 0 -3.110224 -0.850083 2.402315

18 1 0 -2.172627 -1.858848 1.285869

19 1 0 2.664866 0.894611 -0.941646

20 1 0 2.783875 1.043896 0.814652

21 1 0 3.862948 -1.234932 0.919879

22 1 0 3.766534 -1.354916 -0.830293

23 1 0 5.225254 0.679544 -1.039828

24 1 0 5.334958 0.776284 0.707999

25 1 0 7.353547 -0.359473 -0.239795

26 1 0 6.446462 -1.486918 0.771031

27 1 0 6.331171 -1.589431 -0.987614

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.498974 0.000000

3 O 1.210369 2.406687 0.000000

4 O 1.349526 2.376538 2.240081 0.000000

5 C 2.551887 1.517853 3.638858 2.794658 0.000000

6 S 2.725145 1.900302 3.409982 3.365360 2.835946

7 C 4.147763 2.851974 4.864511 4.814327 3.210252

8 S 5.243588 4.004558 6.175302 5.516092 3.773445

9 S 4.928257 3.570488 5.407561 5.873688 3.981151

10 C 6.854260 5.559403 7.659915 7.268134 5.441038

11 C 7.990816 6.753191 8.884336 8.212037 6.442060

12 C 9.342266 8.070304 10.166353 9.653528 7.829303

13 C 10.524690 9.297410 11.411033 10.698053 8.936890

14 H 2.097772 1.088438 2.546541 3.250149 2.165545

15 H 1.880984 3.203337 2.279598 0.971594 3.735287

16 H 3.474388 2.147156 4.482864 3.843570 1.090930

17 H 2.824180 2.159661 3.777823 3.010417 1.094568

18 H 2.848988 2.171588 4.048133 2.588425 1.089844

19 H 6.934659 5.732122 7.613917 7.440366 5.892846

20 H 7.113074 5.713301 7.882815 7.644324 5.532850

21 H 8.094823 6.826967 9.075394 8.221571 6.273588

22 H 7.960144 6.861207 8.862195 8.059004 6.613632

23 H 9.433167 8.216016 10.162565 9.820938 8.174709

24 H 9.559019 8.200668 10.362644 9.963284 7.912828

25 H 11.463085 10.213112 12.308760 11.695858 9.898779

26 H 10.657086 9.404443 11.613161 10.758364 8.870136

27 H 10.539025 9.413640 11.429601 10.620545 9.101293

6 7 8 9 10

6 S 0.000000

7 C 1.758638 0.000000

8 S 2.955071 1.792760 0.000000

9 S 3.055434 1.720931 3.098029 0.000000

10 C 4.345292 2.838869 1.837091 3.411717 0.000000

11 C 5.541937 4.206530 2.762700 4.912543 1.524541

12 C 6.804530 5.367236 4.164847 5.744680 2.532895

13 C 8.040474 6.704959 5.303412 7.211977 3.898879

14 H 2.412577 2.992081 4.433301 3.147971 5.756526

15 H 4.105439 5.664075 6.415529 6.690597 8.147576

16 H 3.009873 2.740275 3.163540 3.322577 4.674397

17 H 3.815934 4.199350 4.791603 4.707115 6.403675

18 H 3.040031 3.565810 3.704613 4.678253 5.500321

19 H 4.271513 2.907829 2.405777 3.417615 1.091964

20 H 4.752011 3.050691 2.414751 3.074231 1.089655

21 H 5.865584 4.533641 2.921454 5.240229 2.157932

22 H 5.502413 4.449797 2.933629 5.448298 2.157148

23 H 6.784456 5.418171 4.461310 5.746734 2.746704

24 H 7.094845 5.502966 4.462494 5.572032 2.762066

25 H 8.928305 7.539378 6.252404 7.889514 4.706337

26 H 8.317666 6.965171 5.439076 7.486636 4.233010

27 H 8.048725 6.894559 5.433675 7.616381 4.220203

11 12 13 14 15

11 C 0.000000

12 C 1.531023 0.000000

13 C 2.544347 1.527285 0.000000

14 H 7.081440 8.282041 9.602754 0.000000

15 H 9.088759 10.524163 11.559699 3.953322 0.000000

16 H 5.690148 7.014976 8.148870 2.474265 4.794673

17 H 7.390667 8.755448 9.849010 2.529984 3.830951

18 H 6.301576 7.771626 8.748097 3.077294 3.534601

19 H 2.170936 2.805716 4.218928 5.873320 8.257942

20 H 2.170231 2.786480 4.215763 5.736407 8.552044

21 H 1.096075 2.157093 2.776241 7.196761 9.131164

22 H 1.095583 2.157549 2.762630 7.319649 8.883595

23 H 2.156469 1.095970 2.157719 8.383484 10.649093

24 H 2.157819 1.095898 2.157888 8.292679 10.864820

25 H 3.498284 2.179157 1.093682 10.453150 12.556627

26 H 2.814701 2.178147 1.094479 9.740864 11.645728

27 H 2.809798 2.177940 1.094387 9.815148 11.438105

16 17 18 19 20

16 H 0.000000

17 H 1.766304 0.000000

18 H 1.769895 1.772892 0.000000

19 H 5.231222 6.897659 5.995390 0.000000

20 H 4.630990 6.391263 5.763236 1.766644 0.000000

21 H 5.474282 7.139388 6.078766 3.071747 2.523594

22 H 6.007143 7.615406 6.325008 2.507278 3.070140

23 H 7.416214 9.147038 8.159715 2.571280 3.087423

24 H 7.003413 8.765665 7.977574 3.140815 2.567297

25 H 9.078134 10.803331 9.763390 4.903984 4.895223

26 H 8.053145 9.715806 8.642458 4.785959 4.452130

27 H 8.412539 10.058738 8.806583 4.428811 4.771360

21 22 23 24 25

21 H 0.000000

22 H 1.756927 0.000000

23 H 3.059664 2.512130 0.000000

24 H 2.501338 3.060769 1.753936 0.000000

25 H 3.780946 3.769119 2.499849 2.502591 0.000000

26 H 2.600037 3.124688 3.076381 2.522201 1.765136

27 H 3.139478 2.580138 2.524683 3.076386 1.765583

26 27

26 H 0.000000

27 H 1.765399 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 7.05D-01

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.119996 -0.411751 -0.156413

2 6 0 -2.833469 0.088874 0.427664

3 8 0 -4.937584 0.275716 -0.725563

4 8 0 -4.276491 -1.745320 -0.021055

5 6 0 -2.360319 -0.628129 1.679027

6 16 0 -1.548883 -0.016800 -0.968696

7 6 0 -0.116047 0.669435 -0.214460

8 16 0 1.109220 -0.573102 0.196407

9 16 0 -0.034743 2.303342 0.319713

10 6 0 2.696701 0.302637 -0.100053

11 6 0 3.864679 -0.669632 0.021371

12 6 0 5.212059 0.022654 -0.200750

13 6 0 6.391132 -0.943323 -0.104442

14 1 0 -2.952434 1.156266 0.604355

15 1 0 -5.116855 -1.979877 -0.448566

16 1 0 -1.434226 -0.174406 2.034860

17 1 0 -3.105210 -0.539065 2.476075

18 1 0 -2.177761 -1.686315 1.492813

19 1 0 2.652932 0.740486 -1.099432

20 1 0 2.783787 1.113729 0.622368

21 1 0 3.857052 -1.136620 1.012959

22 1 0 3.748914 -1.480100 -0.706670

23 1 0 5.212007 0.505245 -1.184750

24 1 0 5.333353 0.825324 0.535459

25 1 0 7.342503 -0.430144 -0.270815

26 1 0 6.438817 -1.415068 0.881999

27 1 0 6.311797 -1.742241 -0.848162

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3327599 0.1919438 0.1796960

Leave Link 202 at Sat Aug 17 17:32:11 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1101.4094680064 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0548790785 Hartrees.

Nuclear repulsion after empirical dispersion term = 1101.3545889278 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2317

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.26D-10

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 88

GePol: Fraction of low-weight points (<1% of avg) = 3.80%

GePol: Cavity surface area = 308.952 Ang\*\*2

GePol: Cavity volume = 319.643 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057090028 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1101.3488799250 Hartrees.

Leave Link 301 at Sat Aug 17 17:32:11 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:32:11 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:32:11 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Lowest energy guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999842 0.017746 -0.000041 -0.000702 Ang= 2.04 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.983213 -0.181811 -0.000812 0.015370 Ang= -21.03 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 7.42D-02

Max alpha theta= 20.403 degrees.

Max beta theta= 20.304 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 17:32:12 2019, MaxMem= 1342177280 cpu: 4.3

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16105467.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.55D-15 for 2295.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.53D-15 for 900 156.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.11D-15 for 2295.

Iteration 1 A^-1\*A deviation from orthogonality is 5.28D-09 for 1045 984.

Iteration 2 A\*A^-1 deviation from unit magnitude is 3.77D-15 for 258.

Iteration 2 A\*A^-1 deviation from orthogonality is 2.82D-15 for 984 68.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 552.

Iteration 2 A^-1\*A deviation from orthogonality is 9.68D-16 for 2285 47.

E= -1658.67603162145

DIIS: error= 2.07D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67603162145 IErMin= 1 ErrMin= 2.07D-03

ErrMax= 2.07D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.38D-03 BMatP= 3.38D-03

IDIUse=3 WtCom= 9.79D-01 WtEn= 2.07D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 88.954 Goal= None Shift= 0.000

Gap= 88.955 Goal= None Shift= 0.000

GapD= 88.954 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=1.40D-04 MaxDP=6.78D-03 OVMax= 8.03D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.39D-04 CP: 1.00D+00

E= -1658.67622965309 Delta-E= -0.000198031638 Rises=F Damp=F

DIIS: error= 2.02D-03 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67622965309 IErMin= 2 ErrMin= 2.02D-03

ErrMax= 2.02D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.26D-03 BMatP= 3.38D-03

IDIUse=3 WtCom= 9.80D-01 WtEn= 2.02D-02

Coeff-Com: 0.494D+00 0.506D+00

Coeff-En: 0.390D+00 0.610D+00

Coeff: 0.492D+00 0.508D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=8.48D-05 MaxDP=5.61D-03 DE=-1.98D-04 OVMax= 7.68D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 7.09D-05 CP: 1.00D+00 6.70D-01

E= -1658.67668644491 Delta-E= -0.000456791821 Rises=F Damp=F

DIIS: error= 8.26D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67668644491 IErMin= 3 ErrMin= 8.26D-04

ErrMax= 8.26D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.79D-04 BMatP= 3.26D-03

IDIUse=3 WtCom= 9.92D-01 WtEn= 8.26D-03

Coeff-Com: 0.455D-01 0.326D+00 0.629D+00

Coeff-En: 0.000D+00 0.221D+00 0.779D+00

Coeff: 0.452D-01 0.325D+00 0.630D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=3.45D-05 MaxDP=1.73D-03 DE=-4.57D-04 OVMax= 3.52D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.92D-05 CP: 1.00D+00 7.91D-01 6.74D-01

E= -1658.67680453466 Delta-E= -0.000118089747 Rises=F Damp=F

DIIS: error= 4.39D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67680453466 IErMin= 4 ErrMin= 4.39D-04

ErrMax= 4.39D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.07D-04 BMatP= 7.79D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 4.39D-03

Coeff-Com: -0.819D-02 0.174D+00 0.403D+00 0.431D+00

Coeff-En: 0.000D+00 0.000D+00 0.566D-01 0.943D+00

Coeff: -0.815D-02 0.174D+00 0.401D+00 0.433D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=1.17D-05 MaxDP=5.45D-04 DE=-1.18D-04 OVMax= 1.31D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.73D-06 CP: 1.00D+00 7.95D-01 7.30D-01 4.79D-01

E= -1658.67682343638 Delta-E= -0.000018901726 Rises=F Damp=F

DIIS: error= 6.39D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67682343638 IErMin= 5 ErrMin= 6.39D-05

ErrMax= 6.39D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.45D-06 BMatP= 1.07D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.677D-02 0.657D-01 0.155D+00 0.222D+00 0.564D+00

Coeff: -0.677D-02 0.657D-01 0.155D+00 0.222D+00 0.564D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=2.30D-06 MaxDP=1.49D-04 DE=-1.89D-05 OVMax= 2.04D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.95D-06 CP: 1.00D+00 7.98D-01 7.27D-01 5.02D-01 7.80D-01

E= -1658.67682399802 Delta-E= -0.000000561639 Rises=F Damp=F

DIIS: error= 1.10D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67682399802 IErMin= 6 ErrMin= 1.10D-05

ErrMax= 1.10D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.08D-07 BMatP= 3.45D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.218D-02 0.158D-01 0.366D-01 0.668D-01 0.259D+00 0.624D+00

Coeff: -0.218D-02 0.158D-01 0.366D-01 0.668D-01 0.259D+00 0.624D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=8.64D-07 MaxDP=4.19D-05 DE=-5.62D-07 OVMax= 7.27D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 6.53D-07 CP: 1.00D+00 7.99D-01 7.26D-01 5.16D-01 8.61D-01

CP: 8.72D-01

E= -1658.67682404396 Delta-E= -0.000000045934 Rises=F Damp=F

DIIS: error= 3.38D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67682404396 IErMin= 7 ErrMin= 3.38D-06

ErrMax= 3.38D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.46D-08 BMatP= 2.08D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.187D-03-0.707D-04-0.986D-03 0.408D-02 0.425D-01 0.233D+00

Coeff-Com: 0.721D+00

Coeff: -0.187D-03-0.707D-04-0.986D-03 0.408D-02 0.425D-01 0.233D+00

Coeff: 0.721D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=4.12D-07 MaxDP=1.42D-05 DE=-4.59D-08 OVMax= 5.45D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 3.02D-07 CP: 1.00D+00 7.99D-01 7.27D-01 5.18D-01 8.86D-01

CP: 9.94D-01 9.53D-01

E= -1658.67682404790 Delta-E= -0.000000003941 Rises=F Damp=F

DIIS: error= 1.27D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67682404790 IErMin= 8 ErrMin= 1.27D-06

ErrMax= 1.27D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.36D-09 BMatP= 1.46D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.250D-03-0.265D-02-0.685D-02-0.869D-02-0.173D-01 0.355D-01

Coeff-Com: 0.426D+00 0.574D+00

Coeff: 0.250D-03-0.265D-02-0.685D-02-0.869D-02-0.173D-01 0.355D-01

Coeff: 0.426D+00 0.574D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=1.86D-07 MaxDP=8.62D-06 DE=-3.94D-09 OVMax= 1.76D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.09D-07 CP: 1.00D+00 7.99D-01 7.27D-01 5.19D-01 9.00D-01

CP: 1.02D+00 1.10D+00 8.05D-01

E= -1658.67682404954 Delta-E= -0.000000001641 Rises=F Damp=F

DIIS: error= 4.67D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67682404954 IErMin= 9 ErrMin= 4.67D-07

ErrMax= 4.67D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.76D-10 BMatP= 5.36D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.136D-03-0.124D-02-0.310D-02-0.456D-02-0.134D-01-0.142D-01

Coeff-Com: 0.113D+00 0.280D+00 0.643D+00

Coeff: 0.136D-03-0.124D-02-0.310D-02-0.456D-02-0.134D-01-0.142D-01

Coeff: 0.113D+00 0.280D+00 0.643D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=1.02D-07 MaxDP=3.69D-06 DE=-1.64D-09 OVMax= 1.48D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 6.38D-08 CP: 1.00D+00 8.00D-01 7.27D-01 5.20D-01 9.07D-01

CP: 1.05D+00 1.16D+00 9.46D-01 9.84D-01

E= -1658.67682404974 Delta-E= -0.000000000198 Rises=F Damp=F

DIIS: error= 3.64D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67682404974 IErMin=10 ErrMin= 3.64D-07

ErrMax= 3.64D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.67D-10 BMatP= 5.76D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.116D-04 0.288D-04 0.167D-03-0.193D-03-0.320D-02-0.217D-01

Coeff-Com: -0.649D-01-0.535D-02 0.448D+00 0.647D+00

Coeff: 0.116D-04 0.288D-04 0.167D-03-0.193D-03-0.320D-02-0.217D-01

Coeff: -0.649D-01-0.535D-02 0.448D+00 0.647D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=5.16D-08 MaxDP=1.97D-06 DE=-1.98D-10 OVMax= 6.76D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.70D-08 CP: 1.00D+00 8.00D-01 7.27D-01 5.20D-01 9.10D-01

CP: 1.05D+00 1.19D+00 1.00D+00 1.22D+00 7.25D-01

E= -1658.67682404982 Delta-E= -0.000000000083 Rises=F Damp=F

DIIS: error= 5.18D-08 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67682404982 IErMin=11 ErrMin= 5.18D-08

ErrMax= 5.18D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.07D-11 BMatP= 2.67D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.142D-04 0.188D-03 0.520D-03 0.600D-03 0.812D-03-0.596D-02

Coeff-Com: -0.391D-01-0.429D-01 0.799D-01 0.224D+00 0.783D+00

Coeff: -0.142D-04 0.188D-03 0.520D-03 0.600D-03 0.812D-03-0.596D-02

Coeff: -0.391D-01-0.429D-01 0.799D-01 0.224D+00 0.783D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=1.79D-08 MaxDP=8.20D-07 DE=-8.32D-11 OVMax= 2.34D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 6.96D-09 CP: 1.00D+00 8.00D-01 7.27D-01 5.20D-01 9.11D-01

CP: 1.06D+00 1.20D+00 1.03D+00 1.28D+00 8.29D-01

CP: 8.62D-01

E= -1658.67682404983 Delta-E= -0.000000000010 Rises=F Damp=F

DIIS: error= 2.91D-08 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.67682404983 IErMin=12 ErrMin= 2.91D-08

ErrMax= 2.91D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.88D-12 BMatP= 1.07D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.743D-05 0.735D-04 0.197D-03 0.264D-03 0.697D-03-0.659D-04

Coeff-Com: -0.821D-02-0.179D-01-0.158D-01 0.154D-01 0.329D+00 0.696D+00

Coeff: -0.743D-05 0.735D-04 0.197D-03 0.264D-03 0.697D-03-0.659D-04

Coeff: -0.821D-02-0.179D-01-0.158D-01 0.154D-01 0.329D+00 0.696D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=4.32D-09 MaxDP=2.12D-07 DE=-9.55D-12 OVMax= 5.90D-07

Error on total polarization charges = 0.04174

SCF Done: E(UB3LYP) = -1658.67682405 A.U. after 12 cycles

NFock= 12 Conv=0.43D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655258695615D+03 PE=-6.145468245471D+03 EE= 1.730183845882D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.58

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:32:37 2019, MaxMem= 1342177280 cpu: 297.3

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 345

Leave Link 701 at Sat Aug 17 17:32:38 2019, MaxMem= 1342177280 cpu: 10.2

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:32:38 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:32:41 2019, MaxMem= 1342177280 cpu: 36.1

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.37982655D+00-2.93880135D+00 5.35397012D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000097194 0.000384674 -0.000034520

2 6 0.001207726 0.001016486 0.000683475

3 8 -0.000438147 0.000562111 -0.000624338

4 8 -0.000392940 -0.000985598 -0.000005502

5 6 0.000283729 0.000281046 -0.000127264

6 16 -0.000119461 -0.000117386 -0.000180734

7 6 0.000320732 -0.001003239 -0.000678335

8 16 -0.000895239 0.000362240 0.000034096

9 16 0.000210424 0.000012697 0.000417993

10 6 0.000122864 -0.000079973 0.000128208

11 6 0.000130092 0.000352723 -0.000089749

12 6 0.000010899 -0.000256613 0.000157626

13 6 -0.000154008 0.000174901 -0.000053790

14 1 -0.000566398 0.000034625 0.000686799

15 1 -0.000363206 -0.000609058 -0.000231272

16 1 0.000100965 0.000069143 -0.000099445

17 1 -0.000233196 -0.000125241 0.000123195

18 1 0.000078370 -0.000338429 -0.000004086

19 1 -0.000143491 0.000100617 -0.000268414

20 1 0.000350351 0.000351244 0.000282347

21 1 0.000024668 -0.000210439 0.000236933

22 1 -0.000047588 -0.000118610 -0.000242347

23 1 -0.000036007 0.000196906 -0.000192850

24 1 0.000023775 0.000170280 0.000220643

25 1 0.000352016 0.000058736 0.000005696

26 1 0.000063124 -0.000173649 0.000219698

27 1 0.000012752 -0.000110195 -0.000364065

-------------------------------------------------------------------

Cartesian Forces: Max 0.001207726 RMS 0.000370703

Leave Link 716 at Sat Aug 17 17:32:42 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.001698677 RMS 0.000337250

Search for a local minimum.

Step number 8 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .33725D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 1 3 4 5 6

8 2

ITU= 0 -1 0 0 -1 -1 0 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.78278.

Iteration 1 RMS(Cart)= 0.03964173 RMS(Int)= 0.00040652

Iteration 2 RMS(Cart)= 0.00073679 RMS(Int)= 0.00000042

Iteration 3 RMS(Cart)= 0.00000020 RMS(Int)= 0.00000042

ITry= 1 IFail=0 DXMaxC= 1.56D-01 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=T

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83265 0.00151 -0.00025 0.00000 -0.00025 2.83240

R2 2.28727 0.00089 0.00329 0.00000 0.00329 2.29055

R3 2.55023 0.00170 0.00071 0.00000 0.00071 2.55094

R4 2.86833 -0.00001 0.00096 0.00000 0.00096 2.86928

R5 3.59105 0.00042 0.00103 0.00000 0.00103 3.59209

R6 2.05685 0.00030 0.00078 0.00000 0.00078 2.05763

R7 1.83605 0.00053 0.00094 0.00000 0.00094 1.83699

R8 2.06156 0.00009 0.00059 0.00000 0.00059 2.06215

R9 2.06843 0.00026 0.00055 0.00000 0.00055 2.06899

R10 2.05951 0.00030 0.00066 0.00000 0.00066 2.06017

R11 3.32334 0.00011 0.00078 0.00000 0.00078 3.32413

R12 3.38782 -0.00060 0.00099 0.00000 0.00099 3.38882

R13 3.25209 0.00018 0.00061 0.00000 0.00061 3.25270

R14 3.47160 0.00077 -0.00034 0.00000 -0.00034 3.47126

R15 2.88096 0.00030 0.00077 0.00000 0.00077 2.88174

R16 2.06351 0.00029 0.00079 0.00000 0.00079 2.06430

R17 2.05915 0.00046 0.00073 0.00000 0.00073 2.05988

R18 2.89321 0.00023 0.00062 0.00000 0.00062 2.89384

R19 2.07128 0.00033 0.00052 0.00000 0.00052 2.07180

R20 2.07035 0.00026 0.00060 0.00000 0.00060 2.07095

R21 2.88615 0.00027 0.00071 0.00000 0.00071 2.88686

R22 2.07108 0.00026 0.00056 0.00000 0.00056 2.07165

R23 2.07095 0.00027 0.00056 0.00000 0.00056 2.07151

R24 2.06676 0.00033 0.00055 0.00000 0.00055 2.06731

R25 2.06827 0.00031 0.00059 0.00000 0.00059 2.06886

R26 2.06809 0.00034 0.00057 0.00000 0.00057 2.06866

A1 2.18130 -0.00017 -0.00023 0.00000 -0.00023 2.18108

A2 1.97194 0.00032 0.00109 0.00000 0.00110 1.97304

A3 2.12951 -0.00014 -0.00076 0.00000 -0.00076 2.12875

A4 2.01642 0.00053 -0.00043 0.00000 -0.00043 2.01598

A5 1.84969 -0.00055 0.00135 0.00000 0.00135 1.85104

A6 1.87231 -0.00004 -0.00001 0.00000 -0.00001 1.87230

A7 1.94852 -0.00009 0.00013 0.00000 0.00013 1.94865

A8 1.94280 -0.00038 -0.00008 0.00000 -0.00008 1.94272

A9 1.82111 0.00053 -0.00097 0.00000 -0.00097 1.82014

A10 1.86997 0.00099 0.00003 0.00000 0.00003 1.86999

A11 1.91459 -0.00023 -0.00081 0.00000 -0.00081 1.91379

A12 1.92811 -0.00003 -0.00056 0.00000 -0.00056 1.92755

A13 1.94982 0.00021 -0.00013 0.00000 -0.00013 1.94968

A14 1.88215 0.00014 0.00050 0.00000 0.00050 1.88265

A15 1.89374 0.00001 0.00032 0.00000 0.00032 1.89406

A16 1.89380 -0.00008 0.00073 0.00000 0.00073 1.89454

A17 1.78638 0.00058 -0.00039 0.00000 -0.00039 1.78599

A18 1.96566 0.00049 -0.00047 0.00000 -0.00047 1.96519

A19 2.14372 0.00022 0.00032 0.00000 0.00032 2.14404

A20 2.15869 -0.00075 0.00141 0.00000 0.00141 2.16011

A21 1.79591 0.00010 -0.00019 0.00000 -0.00019 1.79572

A22 1.92320 0.00020 -0.00003 0.00000 -0.00003 1.92317

A23 1.87989 -0.00017 0.00078 0.00000 0.00078 1.88067

A24 1.89326 0.00017 -0.00062 0.00000 -0.00062 1.89265

A25 1.93834 -0.00003 -0.00017 0.00000 -0.00017 1.93817

A26 1.93979 -0.00021 0.00002 0.00000 0.00002 1.93981

A27 1.88757 0.00004 0.00004 0.00000 0.00004 1.88761

A28 1.95444 0.00017 -0.00012 0.00000 -0.00012 1.95431

A29 1.91605 0.00004 -0.00014 0.00000 -0.00014 1.91591

A30 1.91548 -0.00014 0.00012 0.00000 0.00012 1.91560

A31 1.90712 -0.00014 -0.00006 0.00000 -0.00006 1.90706

A32 1.90824 0.00003 -0.00036 0.00000 -0.00036 1.90788

A33 1.86008 0.00003 0.00060 0.00000 0.00060 1.86068

A34 1.96521 0.00010 -0.00003 0.00000 -0.00003 1.96518

A35 1.90638 -0.00002 -0.00019 0.00000 -0.00019 1.90619

A36 1.90829 -0.00006 -0.00022 0.00000 -0.00022 1.90807

A37 1.91256 -0.00006 -0.00003 0.00000 -0.00003 1.91254

A38 1.91287 0.00002 -0.00013 0.00000 -0.00013 1.91274

A39 1.85526 0.00001 0.00064 0.00000 0.00064 1.85590

A40 1.94463 0.00018 -0.00041 0.00000 -0.00041 1.94422

A41 1.94237 0.00003 -0.00051 0.00000 -0.00051 1.94186

A42 1.94218 -0.00006 -0.00042 0.00000 -0.00042 1.94176

A43 1.87701 -0.00011 0.00059 0.00000 0.00059 1.87761

A44 1.87782 -0.00008 0.00057 0.00000 0.00057 1.87838

A45 1.87654 0.00003 0.00027 0.00000 0.00027 1.87681

D1 2.56409 0.00021 -0.00414 0.00000 -0.00414 2.55996

D2 -1.55157 0.00003 -0.00322 0.00000 -0.00322 -1.55479

D3 0.38630 0.00037 -0.00372 0.00000 -0.00372 0.38258

D4 -0.60842 0.00014 -0.00005 0.00000 -0.00005 -0.60847

D5 1.55910 -0.00005 0.00087 0.00000 0.00087 1.55996

D6 -2.78622 0.00029 0.00037 0.00000 0.00037 -2.78585

D7 -3.11224 0.00006 -0.00184 0.00000 -0.00184 -3.11408

D8 -0.00052 -0.00002 0.00212 0.00000 0.00212 0.00159

D9 -3.11807 -0.00015 0.00124 0.00000 0.00124 -3.11684

D10 -1.04549 -0.00014 0.00101 0.00000 0.00101 -1.04448

D11 1.06444 -0.00013 0.00146 0.00000 0.00146 1.06591

D12 1.05010 0.00026 -0.00034 0.00000 -0.00034 1.04975

D13 3.12268 0.00027 -0.00057 0.00000 -0.00057 3.12210

D14 -1.05057 0.00028 -0.00012 0.00000 -0.00012 -1.05069

D15 -0.97726 -0.00011 0.00083 0.00000 0.00083 -0.97644

D16 1.09532 -0.00010 0.00060 0.00000 0.00060 1.09592

D17 -3.07793 -0.00009 0.00105 0.00000 0.00105 -3.07688

D18 3.08909 0.00030 -0.04821 0.00000 -0.04821 3.04088

D19 -0.98483 0.00052 -0.04772 0.00000 -0.04772 -1.03255

D20 1.11543 0.00034 -0.04834 0.00000 -0.04834 1.06709

D21 1.85157 0.00017 -0.00923 0.00000 -0.00923 1.84235

D22 -1.11014 0.00052 -0.01698 0.00000 -0.01698 -1.12712

D23 2.52674 0.00028 0.00297 0.00000 0.00297 2.52971

D24 -0.79653 0.00004 0.01067 0.00000 0.01067 -0.78586

D25 -3.00895 0.00012 -0.00285 0.00000 -0.00285 -3.01179

D26 -0.89208 0.00009 -0.00259 0.00000 -0.00259 -0.89467

D27 1.14713 0.00014 -0.00245 0.00000 -0.00245 1.14468

D28 -3.12867 -0.00002 -0.00108 0.00000 -0.00108 -3.12975

D29 -1.00706 -0.00005 -0.00134 0.00000 -0.00134 -1.00840

D30 1.03187 -0.00007 -0.00062 0.00000 -0.00062 1.03125

D31 1.07287 0.00008 -0.00192 0.00000 -0.00192 1.07095

D32 -3.08870 0.00005 -0.00218 0.00000 -0.00218 -3.09087

D33 -1.04977 0.00003 -0.00146 0.00000 -0.00146 -1.05123

D34 -1.02937 0.00018 -0.00187 0.00000 -0.00187 -1.03124

D35 1.09224 0.00015 -0.00213 0.00000 -0.00213 1.09012

D36 3.13117 0.00013 -0.00141 0.00000 -0.00141 3.12976

D37 -3.12551 0.00010 -0.00161 0.00000 -0.00161 -3.12711

D38 -0.99653 0.00009 -0.00179 0.00000 -0.00179 -0.99832

D39 1.02696 0.00005 -0.00126 0.00000 -0.00126 1.02570

D40 1.03094 0.00003 -0.00130 0.00000 -0.00130 1.02964

D41 -3.12327 0.00002 -0.00149 0.00000 -0.00149 -3.12476

D42 -1.09978 -0.00002 -0.00096 0.00000 -0.00096 -1.10074

D43 -0.99871 0.00006 -0.00179 0.00000 -0.00179 -1.00050

D44 1.13026 0.00005 -0.00197 0.00000 -0.00197 1.12829

D45 -3.12944 0.00001 -0.00144 0.00000 -0.00144 -3.13088

D46 3.13675 0.00002 -0.00144 0.00000 -0.00144 3.13531

D47 -1.05159 0.00002 -0.00131 0.00000 -0.00131 -1.05290

D48 1.04100 0.00004 -0.00160 0.00000 -0.00160 1.03940

D49 1.01127 0.00001 -0.00116 0.00000 -0.00116 1.01011

D50 3.10612 0.00001 -0.00103 0.00000 -0.00103 3.10509

D51 -1.08447 0.00003 -0.00132 0.00000 -0.00132 -1.08579

D52 -1.01831 0.00002 -0.00184 0.00000 -0.00184 -1.02014

D53 1.07654 0.00002 -0.00171 0.00000 -0.00171 1.07483

D54 -3.11405 0.00004 -0.00200 0.00000 -0.00200 -3.11604

Item Value Threshold Converged?

Maximum Force 0.001699 0.000450 NO

RMS Force 0.000337 0.000300 NO

Maximum Displacement 0.155811 0.001800 NO

RMS Displacement 0.039861 0.001200 NO

Predicted change in Energy=-8.966232D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:32:42 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.117014 -0.359380 -0.182121

2 6 0 -2.818282 0.018275 0.463791

3 8 0 -4.918815 0.425450 -0.640775

4 8 0 -4.309820 -1.694172 -0.240319

5 6 0 -2.365246 -0.884120 1.597747

6 16 0 -1.534215 0.083575 -0.936257

7 6 0 -0.107287 0.694953 -0.108997

8 16 0 1.124313 -0.577772 0.172429

9 16 0 -0.033024 2.268252 0.585214

10 6 0 2.707210 0.334238 -0.019705

11 6 0 3.881505 -0.638289 0.006661

12 6 0 5.225447 0.082175 -0.134018

13 6 0 6.411134 -0.881088 -0.129679

14 1 0 -2.909531 1.052106 0.793127

15 1 0 -5.157158 -1.841798 -0.693296

16 1 0 -1.428188 -0.509467 2.012919

17 1 0 -3.109267 -0.891727 2.400926

18 1 0 -2.209153 -1.908819 1.259884

19 1 0 2.667006 0.875190 -0.967889

20 1 0 2.783914 1.065182 0.785296

21 1 0 3.871856 -1.206095 0.944471

22 1 0 3.775503 -1.369076 -0.803099

23 1 0 5.227702 0.663419 -1.063510

24 1 0 5.336476 0.805461 0.682176

25 1 0 7.359706 -0.346886 -0.237472

26 1 0 6.456602 -1.450486 0.804284

27 1 0 6.340786 -1.600739 -0.951565

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.498843 0.000000

3 O 1.212108 2.407923 0.000000

4 O 1.349900 2.377589 2.241436 0.000000

5 C 2.551857 1.518359 3.639597 2.795718 0.000000

6 S 2.726864 1.900850 3.414631 3.368783 2.836939

7 C 4.146671 2.852276 4.848322 4.835954 3.241115

8 S 5.257843 3.998027 6.179575 5.562958 3.781852

9 S 4.916526 3.582569 5.363760 5.888402 4.049930

10 C 6.861306 5.555598 7.651817 7.307655 5.461718

11 C 8.005606 6.747384 8.887988 8.262789 6.450882

12 C 9.353014 8.066166 10.162710 9.699897 7.845467

13 C 10.541197 9.292103 11.416480 10.752311 8.944767

14 H 2.097955 1.088850 2.546761 3.251286 2.166249

15 H 1.881692 3.204538 2.280346 0.972093 3.736415

16 H 3.474264 2.147247 4.483373 3.845050 1.091243

17 H 2.823309 2.159922 3.776421 3.010219 1.094861

18 H 2.849574 2.172209 4.050133 2.590266 1.090195

19 H 6.940067 5.733446 7.606179 7.470413 5.916183

20 H 7.112530 5.708238 7.859705 7.680297 5.565402

21 H 8.112225 6.818217 9.080245 8.281411 6.279481

22 H 7.981036 6.856221 8.879068 8.111403 6.611206

23 H 9.441752 8.215030 10.158107 9.859016 8.193291

24 H 9.564117 8.195574 10.347251 10.007506 7.937850

25 H 11.476861 10.208652 12.309397 11.747043 9.911173

26 H 10.675433 9.396631 11.619270 10.819723 8.875548

27 H 10.559290 9.408133 11.444677 10.674736 9.099863

6 7 8 9 10

6 S 0.000000

7 C 1.759053 0.000000

8 S 2.955391 1.793284 0.000000

9 S 3.056347 1.721253 3.099947 0.000000

10 C 4.346560 2.838922 1.836911 3.408111 0.000000

11 C 5.544384 4.207299 2.762833 4.909811 1.524950

12 C 6.807100 5.367883 4.165181 5.740013 2.533400

13 C 8.044235 6.706276 5.304125 7.208092 3.899765

14 H 2.412534 2.965461 4.394732 3.129941 5.720474

15 H 4.109965 5.681348 6.465611 6.692073 8.187622

16 H 3.010079 2.774515 3.147591 3.420606 4.684540

17 H 3.816909 4.222458 4.794576 4.769229 6.418243

18 H 3.041088 3.615426 3.750499 4.758008 5.553313

19 H 4.275267 2.909791 2.406517 3.412172 1.092382

20 H 4.751161 3.048913 2.414369 3.069617 1.090041

21 H 5.867367 4.534022 2.922299 5.239107 2.158394

22 H 5.506454 4.451747 2.933705 5.446325 2.157831

23 H 6.787925 5.419796 4.461603 5.741866 2.747866

24 H 7.095550 5.502065 4.462678 5.566030 2.761834

25 H 8.931709 7.540419 6.253116 7.884683 4.707130

26 H 8.320816 6.965747 5.440053 7.482797 4.233455

27 H 8.053122 6.896213 5.433361 7.612899 4.220826

11 12 13 14 15

11 C 0.000000

12 C 1.531352 0.000000

13 C 2.544910 1.527661 0.000000

14 H 7.042310 8.244891 9.563661 0.000000

15 H 9.145261 10.574164 11.621790 3.954234 0.000000

16 H 5.677543 7.016426 8.135342 2.474021 4.796241

17 H 7.393756 8.765950 9.850995 2.530493 3.830235

18 H 6.346726 7.821783 8.791841 3.078225 3.536967

19 H 2.171491 2.805322 4.219669 5.850662 8.287036

20 H 2.170896 2.787925 4.216856 5.693466 8.584718

21 H 1.096351 2.157542 2.776213 7.149098 9.198342

22 H 1.095900 2.157808 2.763725 7.286958 8.945835

23 H 2.156839 1.096269 2.158252 8.355402 10.689176

24 H 2.158165 1.096195 2.158343 8.250441 10.909457

25 H 3.498915 2.179418 1.093975 10.415208 12.614057

26 H 2.815492 2.178349 1.094792 9.694718 11.716454

27 H 2.809372 2.178202 1.094689 9.780077 11.503370

16 17 18 19 20

16 H 0.000000

17 H 1.767116 0.000000

18 H 1.770637 1.773882 0.000000

19 H 5.251010 6.916375 6.040746 0.000000

20 H 4.661370 6.416333 5.831006 1.767321 0.000000

21 H 5.451361 7.138359 6.129599 3.072545 2.523421

22 H 5.978903 7.608791 6.353215 2.508516 3.071133

23 H 7.425695 9.161105 8.204961 2.571216 3.090566

24 H 7.018588 8.784368 8.039750 3.139052 2.567813

25 H 9.072914 10.810060 9.810443 4.903918 4.896720

26 H 8.032199 9.714284 8.689819 4.786482 4.451695

27 H 8.386655 10.052133 8.836678 4.430254 4.772332

21 22 23 24 25

21 H 0.000000

22 H 1.757797 0.000000

23 H 3.060292 2.511519 0.000000

24 H 2.502053 3.061256 1.754830 0.000000

25 H 3.781578 3.769790 2.499699 2.503422 0.000000

26 H 2.600056 3.127075 3.076921 2.521684 1.766009

27 H 3.137883 2.579997 2.525450 3.076938 1.766430

26 27

26 H 0.000000

27 H 1.766068 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 5.31D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.127035 -0.378559 -0.156356

2 6 0 -2.823619 0.052361 0.445262

3 8 0 -4.929430 0.363682 -0.680232

4 8 0 -4.323639 -1.712492 -0.091546

5 6 0 -2.366389 -0.744310 1.654258

6 16 0 -1.547491 -0.014238 -0.961965

7 6 0 -0.114228 0.665564 -0.201773

8 16 0 1.115667 -0.580034 0.187731

9 16 0 -0.031873 2.295358 0.345677

10 6 0 2.699792 0.305732 -0.095481

11 6 0 3.871689 -0.663992 0.012974

12 6 0 5.216663 0.036461 -0.200215

13 6 0 6.399850 -0.926081 -0.114602

14 1 0 -2.910281 1.112189 0.679462

15 1 0 -5.173959 -1.898160 -0.524498

16 1 0 -1.425980 -0.336287 2.028369

17 1 0 -3.105778 -0.676350 2.458874

18 1 0 -2.214911 -1.796023 1.410376

19 1 0 2.655519 0.758117 -1.088802

20 1 0 2.783039 1.106775 0.639087

21 1 0 3.865980 -1.143909 0.998689

22 1 0 3.759117 -1.465221 -0.726185

23 1 0 5.215061 0.530541 -1.178830

24 1 0 5.334280 0.830792 0.546008

25 1 0 7.349168 -0.406886 -0.275881

26 1 0 6.449230 -1.408106 0.867122

27 1 0 6.322889 -1.717437 -0.867048

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3419324 0.1913779 0.1791224

Leave Link 202 at Sat Aug 17 17:32:42 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1100.5296140831 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0547688497 Hartrees.

Nuclear repulsion after empirical dispersion term = 1100.4748452334 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2329

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.94D-09

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 108

GePol: Fraction of low-weight points (<1% of avg) = 4.64%

GePol: Cavity surface area = 309.400 Ang\*\*2

GePol: Cavity volume = 320.027 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0056836150 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1100.4691616183 Hartrees.

Leave Link 301 at Sat Aug 17 17:32:42 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:32:42 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:32:42 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Lowest energy guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999993 0.003796 -0.000010 -0.000149 Ang= 0.44 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999903 -0.013951 0.000030 0.000553 Ang= -1.60 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 2.17D-01

Max alpha theta= 1.441 degrees.

Max beta theta= 1.440 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 17:32:42 2019, MaxMem= 1342177280 cpu: 4.3

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16272723.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.66D-15 for 800.

Iteration 1 A\*A^-1 deviation from orthogonality is 5.04D-15 for 2252 1756.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.22D-15 for 383.

Iteration 1 A^-1\*A deviation from orthogonality is 2.53D-11 for 2306 900.

E= -1658.67682534218

DIIS: error= 2.62D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67682534218 IErMin= 1 ErrMin= 2.62D-05

ErrMax= 2.62D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.46D-07 BMatP= 6.46D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 88.942 Goal= None Shift= 0.000

Gap= 88.944 Goal= None Shift= 0.000

RMSDP=1.81D-06 MaxDP=9.12D-05 OVMax= 1.10D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.80D-06 CP: 1.00D+00

E= -1658.67682537829 Delta-E= -0.000000036106 Rises=F Damp=F

DIIS: error= 2.86D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67682537829 IErMin= 1 ErrMin= 2.62D-05

ErrMax= 2.86D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.91D-07 BMatP= 6.46D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.486D+00 0.514D+00

Coeff: 0.486D+00 0.514D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=1.12D-06 MaxDP=7.86D-05 DE=-3.61D-08 OVMax= 1.05D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 8.85D-07 CP: 1.00D+00 6.19D-01

E= -1658.67682546064 Delta-E= -0.000000082349 Rises=F Damp=F

DIIS: error= 1.17D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67682546064 IErMin= 3 ErrMin= 1.17D-05

ErrMax= 1.17D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.44D-07 BMatP= 5.91D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.458D-01 0.328D+00 0.626D+00

Coeff: 0.458D-01 0.328D+00 0.626D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=4.76D-07 MaxDP=2.73D-05 DE=-8.23D-08 OVMax= 4.72D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.70D-07 CP: 1.00D+00 7.51D-01 6.48D-01

E= -1658.67682548226 Delta-E= -0.000000021621 Rises=F Damp=F

DIIS: error= 5.99D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67682548226 IErMin= 4 ErrMin= 5.99D-06

ErrMax= 5.99D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.03D-08 BMatP= 1.44D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.728D-02 0.176D+00 0.402D+00 0.429D+00

Coeff: -0.728D-02 0.176D+00 0.402D+00 0.429D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=1.64D-07 MaxDP=7.08D-06 DE=-2.16D-08 OVMax= 1.75D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 6.16D-08 CP: 1.00D+00 7.52D-01 7.08D-01 4.74D-01

E= -1658.67682548588 Delta-E= -0.000000003622 Rises=F Damp=F

DIIS: error= 8.56D-07 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67682548588 IErMin= 5 ErrMin= 8.56D-07

ErrMax= 8.56D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.36D-10 BMatP= 2.03D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.639D-02 0.664D-01 0.156D+00 0.219D+00 0.564D+00

Coeff: -0.639D-02 0.664D-01 0.156D+00 0.219D+00 0.564D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=3.29D-08 MaxDP=2.07D-06 DE=-3.62D-09 OVMax= 2.94D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.74D-08 CP: 1.00D+00 7.56D-01 7.07D-01 4.89D-01 7.40D-01

E= -1658.67682548597 Delta-E= -0.000000000088 Rises=F Damp=F

DIIS: error= 1.58D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67682548597 IErMin= 6 ErrMin= 1.58D-07

ErrMax= 1.58D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.32D-11 BMatP= 6.36D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.214D-02 0.162D-01 0.380D-01 0.663D-01 0.266D+00 0.615D+00

Coeff: -0.214D-02 0.162D-01 0.380D-01 0.663D-01 0.266D+00 0.615D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=1.20D-08 MaxDP=5.50D-07 DE=-8.78D-11 OVMax= 1.10D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 8.96D-09 CP: 1.00D+00 7.57D-01 7.06D-01 5.03D-01 8.32D-01

CP: 8.91D-01

E= -1658.67682548598 Delta-E= -0.000000000014 Rises=F Damp=F

DIIS: error= 4.39D-08 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67682548598 IErMin= 7 ErrMin= 4.39D-08

ErrMax= 4.39D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.39D-12 BMatP= 4.32D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.247D-03 0.597D-03 0.908D-03 0.600D-02 0.482D-01 0.219D+00

Coeff-Com: 0.725D+00

Coeff: -0.247D-03 0.597D-03 0.908D-03 0.600D-02 0.482D-01 0.219D+00

Coeff: 0.725D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=5.20D-09 MaxDP=2.46D-07 DE=-1.41D-11 OVMax= 5.29D-07

Error on total polarization charges = 0.04177

SCF Done: E(UB3LYP) = -1658.67682549 A.U. after 7 cycles

NFock= 7 Conv=0.52D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655239665513D+03 PE=-6.143692119971D+03 EE= 1.729306467354D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.57

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:32:58 2019, MaxMem= 1342177280 cpu: 181.6

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 346

Leave Link 701 at Sat Aug 17 17:32:59 2019, MaxMem= 1342177280 cpu: 10.2

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:32:59 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:33:02 2019, MaxMem= 1342177280 cpu: 36.0

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.37127812D+00-2.96546389D+00 4.75662965D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.002136555 0.001844776 -0.000724126

2 6 0.001382257 0.000634715 0.000590913

3 8 0.001527735 -0.001262900 0.000483060

4 8 -0.000382251 -0.000491055 -0.000324061

5 6 0.000128904 0.000527935 -0.000290450

6 16 -0.000228990 0.000113980 -0.000013399

7 6 0.000287199 -0.001077541 -0.000831918

8 16 -0.000858420 0.000644391 0.000033151

9 16 0.000156809 -0.000402230 0.000539894

10 6 0.000364307 0.000058321 0.000155231

11 6 0.000126660 0.000394796 -0.000096530

12 6 0.000008967 -0.000279060 0.000156884

13 6 -0.000299053 0.000230150 -0.000030918

14 1 -0.000519529 -0.000048665 0.000361790

15 1 -0.000048561 -0.000428232 -0.000075622

16 1 -0.000032862 -0.000125652 0.000019232

17 1 -0.000034908 -0.000166979 0.000061251

18 1 0.000016618 -0.000167716 0.000082268

19 1 -0.000177129 -0.000048812 -0.000029820

20 1 0.000351052 0.000191502 0.000056433

21 1 0.000021739 -0.000152447 0.000045479

22 1 -0.000061175 -0.000028517 -0.000047186

23 1 -0.000022254 0.000126487 -0.000001639

24 1 0.000025600 0.000089009 0.000029715

25 1 0.000199482 -0.000081441 0.000029771

26 1 0.000107189 -0.000089781 0.000016999

27 1 0.000097170 -0.000005036 -0.000196400

-------------------------------------------------------------------

Cartesian Forces: Max 0.002136555 RMS 0.000514726

Leave Link 716 at Sat Aug 17 17:33:03 2019, MaxMem= 1342177280 cpu: 0.3

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.002021109 RMS 0.000343841

Search for a local minimum.

Step number 9 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .34384D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 3 4 5 6

2 8 9

ITU= 0 0 -1 0 0 -1 -1 0 0

Eigenvalues --- 0.00234 0.00323 0.00366 0.00400 0.00453

Eigenvalues --- 0.00493 0.00516 0.00745 0.01076 0.01209

Eigenvalues --- 0.02305 0.02766 0.03514 0.03641 0.04637

Eigenvalues --- 0.04832 0.04865 0.04946 0.05451 0.05466

Eigenvalues --- 0.05567 0.05578 0.05690 0.05918 0.08230

Eigenvalues --- 0.08329 0.08774 0.11240 0.12150 0.12210

Eigenvalues --- 0.13943 0.15867 0.16000 0.16000 0.16009

Eigenvalues --- 0.16025 0.16146 0.16576 0.18571 0.19300

Eigenvalues --- 0.19796 0.21908 0.21917 0.22132 0.23328

Eigenvalues --- 0.24614 0.24955 0.24996 0.25247 0.25481

Eigenvalues --- 0.26700 0.29120 0.29347 0.29473 0.29661

Eigenvalues --- 0.30149 0.31419 0.32932 0.33857 0.33875

Eigenvalues --- 0.33888 0.33898 0.34002 0.34032 0.34073

Eigenvalues --- 0.34112 0.34187 0.34412 0.34507 0.34515

Eigenvalues --- 0.34814 0.41032 0.52651 0.57754 5.15403

En-DIIS/RFO-DIIS IScMMF= 0 using points: 9 8

RFO step: Lambda=-4.59579196D-05.

NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=F DC= 1.44D-06 SmlDif= 1.00D-05

RMS Error= 0.1836929263D-02 NUsed= 2 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: -2.02809 3.02809

Iteration 1 RMS(Cart)= 0.13836491 RMS(Int)= 0.00568584

Iteration 2 RMS(Cart)= 0.01086640 RMS(Int)= 0.00010105

Iteration 3 RMS(Cart)= 0.00005056 RMS(Int)= 0.00009940

Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00009940

ITry= 1 IFail=0 DXMaxC= 5.37D-01 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83240 0.00126 0.00075 0.00530 0.00605 2.83846

R2 2.29055 -0.00202 -0.00995 -0.00239 -0.01234 2.27821

R3 2.55094 0.00104 -0.00214 0.00230 0.00016 2.55110

R4 2.86928 -0.00017 -0.00290 -0.00113 -0.00403 2.86525

R5 3.59209 0.00024 -0.00313 0.00107 -0.00207 3.59002

R6 2.05763 0.00011 -0.00236 -0.00014 -0.00250 2.05513

R7 1.83699 0.00012 -0.00286 -0.00011 -0.00297 1.83402

R8 2.06215 -0.00004 -0.00179 -0.00053 -0.00232 2.05983

R9 2.06899 0.00008 -0.00168 0.00018 -0.00150 2.06749

R10 2.06017 0.00009 -0.00201 -0.00002 -0.00202 2.05815

R11 3.32413 -0.00002 -0.00237 -0.00018 -0.00255 3.32158

R12 3.38882 -0.00073 -0.00300 -0.00271 -0.00572 3.38310

R13 3.25270 -0.00017 -0.00184 0.00048 -0.00136 3.25134

R14 3.47126 0.00079 0.00103 0.00324 0.00427 3.47553

R15 2.88174 0.00007 -0.00234 0.00019 -0.00215 2.87959

R16 2.06430 0.00002 -0.00239 0.00003 -0.00236 2.06194

R17 2.05988 0.00018 -0.00221 0.00042 -0.00179 2.05809

R18 2.89384 0.00007 -0.00188 0.00008 -0.00180 2.89203

R19 2.07180 0.00013 -0.00158 0.00037 -0.00121 2.07059

R20 2.07095 0.00005 -0.00181 0.00011 -0.00171 2.06925

R21 2.88686 0.00007 -0.00215 0.00013 -0.00202 2.88484

R22 2.07165 0.00007 -0.00171 0.00017 -0.00154 2.07011

R23 2.07151 0.00007 -0.00170 0.00018 -0.00152 2.06999

R24 2.06731 0.00013 -0.00168 0.00035 -0.00133 2.06599

R25 2.06886 0.00009 -0.00179 0.00028 -0.00151 2.06734

R26 2.06866 0.00013 -0.00173 0.00032 -0.00140 2.06726

A1 2.18108 -0.00010 0.00068 -0.00050 0.00015 2.18123

A2 1.97304 0.00011 -0.00332 -0.00007 -0.00342 1.96962

A3 2.12875 -0.00001 0.00231 0.00048 0.00276 2.13151

A4 2.01598 0.00039 0.00131 0.00122 0.00251 2.01850

A5 1.85104 -0.00050 -0.00407 -0.00474 -0.00882 1.84222

A6 1.87230 -0.00007 0.00002 0.00074 0.00077 1.87308

A7 1.94865 0.00011 -0.00039 -0.00202 -0.00242 1.94623

A8 1.94272 -0.00028 0.00024 -0.00235 -0.00211 1.94061

A9 1.82014 0.00035 0.00292 0.00786 0.01080 1.83094

A10 1.86999 0.00083 -0.00008 0.00611 0.00603 1.87602

A11 1.91379 0.00005 0.00245 -0.00153 0.00092 1.91470

A12 1.92755 0.00005 0.00170 0.00052 0.00223 1.92978

A13 1.94968 0.00020 0.00040 0.00216 0.00255 1.95224

A14 1.88265 -0.00005 -0.00152 0.00022 -0.00129 1.88136

A15 1.89406 -0.00011 -0.00097 -0.00054 -0.00151 1.89255

A16 1.89454 -0.00015 -0.00222 -0.00091 -0.00313 1.89141

A17 1.78599 0.00033 0.00119 0.00305 0.00424 1.79023

A18 1.96519 0.00104 0.00142 0.00074 0.00154 1.96672

A19 2.14404 0.00004 -0.00097 -0.00160 -0.00321 2.14083

A20 2.16011 -0.00116 -0.00428 -0.00588 -0.01078 2.14933

A21 1.79572 0.00010 0.00057 0.00064 0.00121 1.79693

A22 1.92317 0.00026 0.00010 0.00124 0.00134 1.92451

A23 1.88067 -0.00027 -0.00235 -0.00182 -0.00417 1.87650

A24 1.89265 0.00021 0.00187 0.00232 0.00419 1.89684

A25 1.93817 0.00003 0.00052 0.00021 0.00073 1.93889

A26 1.93981 -0.00027 -0.00005 -0.00160 -0.00166 1.93815

A27 1.88761 0.00004 -0.00012 -0.00032 -0.00045 1.88717

A28 1.95431 0.00011 0.00038 0.00080 0.00118 1.95549

A29 1.91591 0.00004 0.00043 -0.00001 0.00042 1.91633

A30 1.91560 -0.00010 -0.00036 -0.00014 -0.00050 1.91510

A31 1.90706 -0.00009 0.00018 -0.00101 -0.00083 1.90624

A32 1.90788 0.00006 0.00110 0.00094 0.00203 1.90991

A33 1.86068 -0.00001 -0.00182 -0.00065 -0.00247 1.85820

A34 1.96518 0.00010 0.00008 0.00065 0.00073 1.96592

A35 1.90619 -0.00002 0.00058 -0.00001 0.00057 1.90676

A36 1.90807 -0.00003 0.00067 -0.00013 0.00054 1.90861

A37 1.91254 -0.00004 0.00008 -0.00008 0.00000 1.91254

A38 1.91274 0.00000 0.00040 0.00033 0.00073 1.91347

A39 1.85590 -0.00002 -0.00192 -0.00085 -0.00278 1.85312

A40 1.94422 0.00021 0.00125 0.00138 0.00263 1.94685

A41 1.94186 0.00009 0.00155 0.00062 0.00217 1.94402

A42 1.94176 0.00003 0.00126 0.00021 0.00147 1.94323

A43 1.87761 -0.00017 -0.00180 -0.00137 -0.00318 1.87443

A44 1.87838 -0.00014 -0.00172 -0.00105 -0.00277 1.87562

A45 1.87681 -0.00004 -0.00081 0.00007 -0.00074 1.87607

D1 2.55996 0.00014 0.01253 0.01978 0.03230 2.59226

D2 -1.55479 0.00015 0.00975 0.01431 0.02406 -1.53073

D3 0.38258 0.00030 0.01126 0.02142 0.03268 0.41526

D4 -0.60847 -0.00010 0.00015 0.01616 0.01631 -0.59216

D5 1.55996 -0.00009 -0.00263 0.01069 0.00807 1.56803

D6 -2.78585 0.00005 -0.00112 0.01780 0.01669 -2.76916

D7 -3.11408 0.00014 0.00557 0.00373 0.00931 -3.10477

D8 0.00159 -0.00010 -0.00641 0.00021 -0.00621 -0.00461

D9 -3.11684 -0.00007 -0.00375 -0.00316 -0.00691 -3.12374

D10 -1.04448 -0.00007 -0.00305 -0.00351 -0.00656 -1.05105

D11 1.06591 -0.00010 -0.00443 -0.00286 -0.00728 1.05862

D12 1.04975 0.00022 0.00104 0.00389 0.00493 1.05469

D13 3.12210 0.00022 0.00173 0.00354 0.00528 3.12738

D14 -1.05069 0.00019 0.00036 0.00420 0.00456 -1.04613

D15 -0.97644 -0.00011 -0.00251 -0.00315 -0.00566 -0.98209

D16 1.09592 -0.00011 -0.00182 -0.00350 -0.00531 1.09060

D17 -3.07688 -0.00013 -0.00319 -0.00284 -0.00604 -3.08291

D18 3.04088 0.00033 0.14599 0.03089 0.17685 -3.06546

D19 -1.03255 0.00053 0.14450 0.02774 0.17225 -0.86030

D20 1.06709 0.00046 0.14636 0.02864 0.17502 1.24212

D21 1.84235 0.00035 0.02794 -0.02559 0.00234 1.84469

D22 -1.12712 0.00093 0.05142 0.01644 0.06787 -1.05926

D23 2.52971 0.00026 -0.00898 0.05437 0.04524 2.57495

D24 -0.78586 -0.00019 -0.03232 0.01240 -0.01977 -0.80563

D25 -3.01179 0.00000 0.00863 -0.02697 -0.01834 -3.03013

D26 -0.89467 0.00002 0.00785 -0.02711 -0.01926 -0.91393

D27 1.14468 0.00004 0.00743 -0.02724 -0.01982 1.12486

D28 -3.12975 -0.00007 0.00327 0.01180 0.01508 -3.11468

D29 -1.00840 -0.00009 0.00406 0.01105 0.01511 -0.99329

D30 1.03125 -0.00014 0.00188 0.01017 0.01206 1.04331

D31 1.07095 0.00007 0.00581 0.01314 0.01895 1.08990

D32 -3.09087 0.00006 0.00659 0.01238 0.01898 -3.07190

D33 -1.05123 0.00000 0.00442 0.01151 0.01593 -1.03530

D34 -1.03124 0.00018 0.00565 0.01449 0.02014 -1.01110

D35 1.09012 0.00017 0.00644 0.01373 0.02017 1.11029

D36 3.12976 0.00012 0.00426 0.01286 0.01712 -3.13630

D37 -3.12711 0.00007 0.00486 0.00564 0.01050 -3.11661

D38 -0.99832 0.00007 0.00543 0.00597 0.01140 -0.98693

D39 1.02570 0.00002 0.00382 0.00487 0.00869 1.03439

D40 1.02964 0.00001 0.00394 0.00582 0.00977 1.03940

D41 -3.12476 0.00001 0.00451 0.00616 0.01066 -3.11410

D42 -1.10074 -0.00004 0.00290 0.00506 0.00795 -1.09279

D43 -1.00050 0.00004 0.00541 0.00665 0.01206 -0.98844

D44 1.12829 0.00005 0.00598 0.00698 0.01296 1.14124

D45 -3.13088 -0.00001 0.00437 0.00588 0.01025 -3.12063

D46 3.13531 0.00002 0.00436 0.00574 0.01010 -3.13778

D47 -1.05290 0.00000 0.00397 0.00535 0.00932 -1.04358

D48 1.03940 0.00004 0.00484 0.00600 0.01084 1.05025

D49 1.01011 0.00000 0.00352 0.00536 0.00888 1.01899

D50 3.10509 -0.00001 0.00313 0.00497 0.00810 3.11319

D51 -1.08579 0.00002 0.00400 0.00562 0.00962 -1.07617

D52 -1.02014 0.00005 0.00556 0.00625 0.01181 -1.00833

D53 1.07483 0.00003 0.00517 0.00586 0.01103 1.08587

D54 -3.11604 0.00007 0.00604 0.00651 0.01255 -3.10349

Item Value Threshold Converged?

Maximum Force 0.002021 0.000450 NO

RMS Force 0.000344 0.000300 NO

Maximum Displacement 0.536695 0.001800 NO

RMS Displacement 0.144091 0.001200 NO

Predicted change in Energy=-2.109271D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:33:03 2019, MaxMem= 1342177280 cpu: 0.6

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.093186 -0.459383 -0.196538

2 6 0 -2.846537 0.086154 0.439386

3 8 0 -4.955737 0.207971 -0.710404

4 8 0 -4.139396 -1.808539 -0.186826

5 6 0 -2.299691 -0.714853 1.604844

6 16 0 -1.576712 0.225788 -0.966714

7 6 0 -0.124857 0.742278 -0.121212

8 16 0 1.081053 -0.570389 0.045271

9 16 0 -0.040095 2.215429 0.763591

10 6 0 2.683142 0.330144 -0.024734

11 6 0 3.843011 -0.657681 -0.054842

12 6 0 5.199772 0.050062 -0.075232

13 6 0 6.371136 -0.926723 -0.140675

14 1 0 -3.054670 1.112880 0.731323

15 1 0 -4.953429 -2.075768 -0.642736

16 1 0 -1.410394 -0.225460 2.002063

17 1 0 -3.037282 -0.773355 2.410774

18 1 0 -2.032266 -1.728645 1.310058

19 1 0 2.672263 0.950402 -0.922359

20 1 0 2.751782 0.987732 0.840712

21 1 0 3.792668 -1.315924 0.819665

22 1 0 3.755768 -1.303444 -0.934841

23 1 0 5.239863 0.729412 -0.933659

24 1 0 5.294513 0.679158 0.816477

25 1 0 7.330682 -0.402872 -0.150511

26 1 0 6.375955 -1.602029 0.719997

27 1 0 6.324804 -1.543982 -1.042653

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.502046 0.000000

3 O 1.205576 2.405323 0.000000

4 O 1.349982 2.377706 2.237601 0.000000

5 C 2.554773 1.516227 3.642328 2.791191 0.000000

6 S 2.719425 1.899755 3.388778 3.363638 2.832034

7 C 4.146963 2.855226 4.895920 4.756837 3.135667

8 S 5.181075 4.001542 6.133491 5.370286 3.725932

9 S 4.950153 3.537661 5.510543 5.822361 3.794738

10 C 6.824331 5.554484 7.670563 7.151732 5.345668

11 C 7.939939 6.748897 8.865499 8.066023 6.363224

12 C 9.307702 8.062830 10.176577 9.522967 7.723321

13 C 10.474902 9.291280 11.397814 10.547560 8.847314

14 H 2.100345 1.087526 2.551762 3.248740 2.161860

15 H 1.884625 3.206850 2.284743 0.970522 3.734439

16 H 3.476484 2.145127 4.484952 3.839899 1.090017

17 H 2.830474 2.159053 3.792785 3.005626 1.094069

18 H 2.851009 2.171314 4.047151 2.585932 1.089124

19 H 6.948785 5.749646 7.666975 7.385897 5.820667

20 H 7.072737 5.684635 7.900621 7.507549 5.385171

21 H 7.997063 6.796284 9.010990 8.010826 6.172085

22 H 7.928658 6.885486 8.844494 7.946589 6.592801

23 H 9.437287 8.227327 10.211366 9.745228 8.085467

24 H 9.510593 8.171325 10.374054 9.807849 7.761233

25 H 11.424101 10.206024 12.314329 11.555947 9.794013

26 H 10.571121 9.379929 11.564142 10.556401 8.765665

27 H 10.508414 9.432247 11.420609 10.502472 9.059724

6 7 8 9 10

6 S 0.000000

7 C 1.757703 0.000000

8 S 2.953256 1.790259 0.000000

9 S 3.051856 1.720534 3.087675 0.000000

10 C 4.364009 2.839722 1.839171 3.404670 0.000000

11 C 5.566456 4.208119 2.765151 4.899297 1.523811

12 C 6.837131 5.369632 4.166933 5.731374 2.532671

13 C 8.073346 6.707001 5.305331 7.196854 3.898007

14 H 2.419632 3.073754 4.517550 3.210034 5.840101

15 H 4.099309 5.615022 6.257354 6.673304 8.030414

16 H 3.007478 2.664099 3.186741 3.060960 4.601482

17 H 3.813001 4.146121 4.753681 4.541935 6.314480

18 H 3.034968 3.433978 3.554433 4.452313 5.315576

19 H 4.310548 2.917025 2.404384 3.435056 1.091133

20 H 4.752179 3.043122 2.419050 3.050863 1.089095

21 H 5.865004 4.524207 2.916910 5.211878 2.157220

22 H 5.547514 4.461639 2.941444 5.447542 2.155790

23 H 6.835234 5.425906 4.465814 5.741678 2.742697

24 H 7.113301 5.500256 4.461993 5.551664 2.765630

25 H 8.966776 7.543029 6.254939 7.875242 4.706672

26 H 8.332516 6.961607 5.436500 7.465962 4.233767

27 H 8.097642 6.904648 5.443196 7.609706 4.220214

11 12 13 14 15

11 C 0.000000

12 C 1.530397 0.000000

13 C 2.543849 1.526593 0.000000

14 H 7.164561 8.361574 9.683293 0.000000

15 H 8.929386 10.388873 11.393776 3.957372 0.000000

16 H 5.658262 6.934361 8.101562 2.471756 4.792879

17 H 7.309656 8.643339 9.749449 2.525616 3.832991

18 H 6.126075 7.575302 8.565329 3.074818 3.530877

19 H 2.170062 2.813634 4.220934 5.963122 8.208963

20 H 2.167990 2.776839 4.210461 5.808830 8.423533

21 H 1.095710 2.155621 2.778890 7.265874 8.900010

22 H 1.094997 2.157788 2.759124 7.415982 8.748253

23 H 2.155816 1.095455 2.156707 8.468677 10.576241

24 H 2.157126 1.095392 2.157339 8.360875 10.711640

25 H 3.498275 2.179815 1.093273 10.532363 12.407266

26 H 2.812112 2.178348 1.093992 9.813641 11.420876

27 H 2.814355 2.177745 1.093946 9.908603 11.297843

16 17 18 19 20

16 H 0.000000

17 H 1.764653 0.000000

18 H 1.767812 1.770371 0.000000

19 H 5.157808 6.832278 5.856072 0.000000

20 H 4.488238 6.251382 5.521422 1.765258 0.000000

21 H 5.446010 7.033792 5.860092 3.070210 2.527987

22 H 6.039593 7.590762 6.222677 2.500792 3.067582

23 H 7.331860 9.052882 7.997510 2.577117 3.066867

24 H 6.868750 8.606416 7.728055 3.158056 2.561502

25 H 9.003969 10.686072 9.568476 4.912022 4.886986

26 H 8.010360 9.599712 8.429851 4.788483 4.456015

27 H 8.416773 10.008430 8.683891 4.424644 4.766878

21 22 23 24 25

21 H 0.000000

22 H 1.754938 0.000000

23 H 3.058091 2.516951 0.000000

24 H 2.497180 3.060320 1.751710 0.000000

25 H 3.780536 3.769113 2.503380 2.500367 0.000000

26 H 2.600993 3.113361 3.075858 2.526389 1.762744

27 H 3.151500 2.582523 2.521368 3.075746 1.763475

26 27

26 H 0.000000

27 H 1.764347 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.44D-01

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.096672 -0.489509 -0.108379

2 6 0 -2.844456 0.163184 0.403567

3 8 0 -4.960970 0.070153 -0.735421

4 8 0 -4.146172 -1.811596 0.160116

5 6 0 -2.291840 -0.401555 1.697642

6 16 0 -1.583697 0.025930 -1.010901

7 6 0 -0.124953 0.689532 -0.288947

8 16 0 1.078772 -0.571345 0.118810

9 16 0 -0.030626 2.304663 0.296452

10 6 0 2.682593 0.293096 -0.132285

11 6 0 3.839776 -0.686484 0.020527

12 6 0 5.198126 -0.000831 -0.143423

13 6 0 6.366595 -0.976394 -0.027476

14 1 0 -3.048082 1.227600 0.494483

15 1 0 -4.963890 -2.158244 -0.231147

16 1 0 -1.398698 0.151601 1.988250

17 1 0 -3.024182 -0.301717 2.504298

18 1 0 -2.028910 -1.454045 1.601089

19 1 0 2.667269 0.729795 -1.132100

20 1 0 2.758641 1.104147 0.590586

21 1 0 3.793631 -1.164668 1.005307

22 1 0 3.745058 -1.488650 -0.718783

23 1 0 5.234179 0.501189 -1.116407

24 1 0 5.300379 0.787195 0.610529

25 1 0 7.327354 -0.467718 -0.143396

26 1 0 6.375477 -1.474181 0.946663

27 1 0 6.312711 -1.754951 -0.794069

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3150640 0.1940034 0.1815039

Leave Link 202 at Sat Aug 17 17:33:03 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1104.4378659356 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0552461548 Hartrees.

Nuclear repulsion after empirical dispersion term = 1104.3826197807 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2314

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.11D-10

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 99

GePol: Fraction of low-weight points (<1% of avg) = 4.28%

GePol: Cavity surface area = 308.336 Ang\*\*2

GePol: Cavity volume = 319.724 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0056060334 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1104.3770137473 Hartrees.

Leave Link 301 at Sat Aug 17 17:33:03 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.84D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:33:03 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:33:03 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999348 0.036047 -0.001118 -0.001943 Ang= 4.14 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.63061334876

Leave Link 401 at Sat Aug 17 17:33:04 2019, MaxMem= 1342177280 cpu: 7.5

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16063788.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.55D-15 for 579.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.20D-15 for 708 444.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.44D-15 for 189.

Iteration 1 A^-1\*A deviation from orthogonality is 4.26D-12 for 938 923.

E= -1658.63517825988

DIIS: error= 6.35D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.63517825988 IErMin= 1 ErrMin= 6.35D-03

ErrMax= 6.35D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.04D-01 BMatP= 1.04D-01

IDIUse=3 WtCom= 9.37D-01 WtEn= 6.35D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.430 Goal= None Shift= 0.000

Gap= 0.484 Goal= None Shift= 0.000

GapD= 0.430 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=6.97D-04 MaxDP=1.62D-02 OVMax= 4.40D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 6.96D-04 CP: 9.98D-01

E= -1658.67593154047 Delta-E= -0.040753280594 Rises=F Damp=F

DIIS: error= 1.19D-03 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67593154047 IErMin= 2 ErrMin= 1.19D-03

ErrMax= 1.19D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.12D-03 BMatP= 1.04D-01

IDIUse=3 WtCom= 9.88D-01 WtEn= 1.19D-02

Coeff-Com: -0.455D-01 0.105D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.449D-01 0.104D+01

Gap= 0.124 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=1.19D-04 MaxDP=4.84D-03 DE=-4.08D-02 OVMax= 7.03D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.15D-04 CP: 9.98D-01 1.05D+00

E= -1658.67602284660 Delta-E= -0.000091306123 Rises=F Damp=F

DIIS: error= 1.81D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67602284660 IErMin= 2 ErrMin= 1.19D-03

ErrMax= 1.81D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.83D-03 BMatP= 2.12D-03

IDIUse=3 WtCom= 1.90D-01 WtEn= 8.10D-01

Coeff-Com: -0.392D-01 0.587D+00 0.452D+00

Coeff-En: 0.000D+00 0.440D+00 0.560D+00

Coeff: -0.746D-02 0.468D+00 0.540D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=7.54D-05 MaxDP=4.66D-03 DE=-9.13D-05 OVMax= 5.35D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 4.43D-05 CP: 9.98D-01 1.07D+00 4.90D-01

E= -1658.67642741298 Delta-E= -0.000404566383 Rises=F Damp=F

DIIS: error= 8.12D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67642741298 IErMin= 4 ErrMin= 8.12D-04

ErrMax= 8.12D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.99D-04 BMatP= 2.12D-03

IDIUse=3 WtCom= 9.92D-01 WtEn= 8.12D-03

Coeff-Com: -0.111D-01 0.138D+00 0.331D+00 0.542D+00

Coeff-En: 0.000D+00 0.000D+00 0.184D+00 0.816D+00

Coeff: -0.110D-01 0.137D+00 0.330D+00 0.545D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=2.59D-05 MaxDP=1.70D-03 DE=-4.05D-04 OVMax= 2.60D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.52D-05 CP: 9.98D-01 1.08D+00 6.25D-01 6.90D-01

E= -1658.67652899113 Delta-E= -0.000101578150 Rises=F Damp=F

DIIS: error= 1.58D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67652899113 IErMin= 5 ErrMin= 1.58D-04

ErrMax= 1.58D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.78D-05 BMatP= 5.99D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.58D-03

Coeff-Com: -0.388D-02 0.410D-01 0.162D+00 0.314D+00 0.487D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.387D-02 0.409D-01 0.162D+00 0.313D+00 0.488D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=5.93D-06 MaxDP=2.88D-04 DE=-1.02D-04 OVMax= 6.81D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 4.87D-06 CP: 9.98D-01 1.08D+00 6.32D-01 7.42D-01 8.49D-01

E= -1658.67653205620 Delta-E= -0.000003065068 Rises=F Damp=F

DIIS: error= 5.99D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67653205620 IErMin= 6 ErrMin= 5.99D-05

ErrMax= 5.99D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.88D-06 BMatP= 1.78D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.183D-03-0.877D-02 0.237D-01 0.712D-01 0.300D+00 0.614D+00

Coeff: 0.183D-03-0.877D-02 0.237D-01 0.712D-01 0.300D+00 0.614D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=3.14D-06 MaxDP=1.26D-04 DE=-3.07D-06 OVMax= 2.43D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.34D-06 CP: 9.98D-01 1.08D+00 6.42D-01 7.66D-01 9.06D-01

CP: 7.78D-01

E= -1658.67653265388 Delta-E= -0.000000597680 Rises=F Damp=F

DIIS: error= 1.39D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67653265388 IErMin= 7 ErrMin= 1.39D-05

ErrMax= 1.39D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.05D-07 BMatP= 2.88D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.626D-03-0.102D-01-0.106D-01-0.754D-02 0.764D-01 0.301D+00

Coeff-Com: 0.650D+00

Coeff: 0.626D-03-0.102D-01-0.106D-01-0.754D-02 0.764D-01 0.301D+00

Coeff: 0.650D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=1.41D-06 MaxDP=5.45D-05 DE=-5.98D-07 OVMax= 1.37D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.11D-06 CP: 9.98D-01 1.08D+00 6.44D-01 7.75D-01 9.38D-01

CP: 8.92D-01 9.63D-01

E= -1658.67653274339 Delta-E= -0.000000089513 Rises=F Damp=F

DIIS: error= 3.94D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67653274339 IErMin= 8 ErrMin= 3.94D-06

ErrMax= 3.94D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.96D-08 BMatP= 3.05D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.182D-03-0.187D-02-0.790D-02-0.153D-01-0.270D-01-0.184D-02

Coeff-Com: 0.262D+00 0.792D+00

Coeff: 0.182D-03-0.187D-02-0.790D-02-0.153D-01-0.270D-01-0.184D-02

Coeff: 0.262D+00 0.792D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=7.24D-07 MaxDP=2.77D-05 DE=-8.95D-08 OVMax= 6.77D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 3.49D-07 CP: 9.98D-01 1.08D+00 6.44D-01 7.80D-01 9.54D-01

CP: 9.43D-01 1.16D+00 1.01D+00

E= -1658.67653276008 Delta-E= -0.000000016692 Rises=F Damp=F

DIIS: error= 1.90D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67653276008 IErMin= 9 ErrMin= 1.90D-06

ErrMax= 1.90D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.94D-09 BMatP= 3.96D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.764D-05 0.693D-03-0.201D-02-0.594D-02-0.228D-01-0.444D-01

Coeff-Com: 0.108D-01 0.323D+00 0.741D+00

Coeff: -0.764D-05 0.693D-03-0.201D-02-0.594D-02-0.228D-01-0.444D-01

Coeff: 0.108D-01 0.323D+00 0.741D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=2.90D-07 MaxDP=1.35D-05 DE=-1.67D-08 OVMax= 2.99D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.36D-07 CP: 9.98D-01 1.08D+00 6.45D-01 7.80D-01 9.58D-01

CP: 9.59D-01 1.22D+00 1.17D+00 8.25D-01

E= -1658.67653276211 Delta-E= -0.000000002027 Rises=F Damp=F

DIIS: error= 8.74D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67653276211 IErMin=10 ErrMin= 8.74D-07

ErrMax= 8.74D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.53D-09 BMatP= 5.94D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.265D-04 0.605D-03-0.832D-04-0.123D-02-0.816D-02-0.234D-01

Coeff-Com: -0.315D-01 0.578D-01 0.408D+00 0.598D+00

Coeff: -0.265D-04 0.605D-03-0.832D-04-0.123D-02-0.816D-02-0.234D-01

Coeff: -0.315D-01 0.578D-01 0.408D+00 0.598D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=9.74D-08 MaxDP=4.59D-06 DE=-2.03D-09 OVMax= 9.41D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 5.07D-08 CP: 9.98D-01 1.08D+00 6.45D-01 7.81D-01 9.58D-01

CP: 9.63D-01 1.24D+00 1.19D+00 9.39D-01 7.55D-01

E= -1658.67653276252 Delta-E= -0.000000000412 Rises=F Damp=F

DIIS: error= 2.24D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67653276252 IErMin=11 ErrMin= 2.24D-07

ErrMax= 2.24D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.33D-10 BMatP= 1.53D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.127D-04 0.255D-03 0.720D-04-0.263D-03-0.249D-02-0.859D-02

Coeff-Com: -0.166D-01 0.591D-02 0.162D+00 0.313D+00 0.547D+00

Coeff: -0.127D-04 0.255D-03 0.720D-04-0.263D-03-0.249D-02-0.859D-02

Coeff: -0.166D-01 0.591D-02 0.162D+00 0.313D+00 0.547D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=3.44D-08 MaxDP=1.40D-06 DE=-4.12D-10 OVMax= 4.09D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 2.72D-08 CP: 9.98D-01 1.08D+00 6.45D-01 7.81D-01 9.58D-01

CP: 9.62D-01 1.24D+00 1.20D+00 9.68D-01 8.07D-01

CP: 7.68D-01

E= -1658.67653276253 Delta-E= -0.000000000012 Rises=F Damp=F

DIIS: error= 1.15D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.67653276253 IErMin=12 ErrMin= 1.15D-07

ErrMax= 1.15D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.02D-11 BMatP= 1.33D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.567D-06-0.162D-04 0.795D-04 0.217D-03 0.968D-03 0.171D-02

Coeff-Com: -0.174D-02-0.160D-01-0.167D-01 0.290D-01 0.372D+00 0.630D+00

Coeff: -0.567D-06-0.162D-04 0.795D-04 0.217D-03 0.968D-03 0.171D-02

Coeff: -0.174D-02-0.160D-01-0.167D-01 0.290D-01 0.372D+00 0.630D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=1.58D-08 MaxDP=6.28D-07 DE=-1.18D-11 OVMax= 1.65D-06

Cycle 13 Pass 1 IDiag 1:

RMSU= 7.57D-09 CP: 9.98D-01 1.08D+00 6.45D-01 7.81D-01 9.58D-01

CP: 9.63D-01 1.24D+00 1.20D+00 9.75D-01 8.46D-01

CP: 9.62D-01 8.11D-01

E= -1658.67653276255 Delta-E= -0.000000000022 Rises=F Damp=F

DIIS: error= 3.77D-08 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1658.67653276255 IErMin=13 ErrMin= 3.77D-08

ErrMax= 3.77D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.52D-12 BMatP= 4.02D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.114D-05-0.322D-04 0.204D-04 0.104D-03 0.606D-03 0.154D-02

Coeff-Com: 0.122D-02-0.638D-02-0.230D-01-0.223D-01 0.712D-01 0.202D+00

Coeff-Com: 0.775D+00

Coeff: 0.114D-05-0.322D-04 0.204D-04 0.104D-03 0.606D-03 0.154D-02

Coeff: 0.122D-02-0.638D-02-0.230D-01-0.223D-01 0.712D-01 0.202D+00

Coeff: 0.775D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=5.26D-09 MaxDP=2.61D-07 DE=-2.23D-11 OVMax= 6.17D-07

Error on total polarization charges = 0.04164

SCF Done: E(UB3LYP) = -1658.67653276 A.U. after 13 cycles

NFock= 13 Conv=0.53D-08 -V/T= 2.0020

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655297482171D+03 PE=-6.151580005844D+03 EE= 1.733228977163D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.52

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:33:31 2019, MaxMem= 1342177280 cpu: 315.1

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 332

Leave Link 701 at Sat Aug 17 17:33:32 2019, MaxMem= 1342177280 cpu: 10.2

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:33:32 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:33:35 2019, MaxMem= 1342177280 cpu: 36.3

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.42699175D+00-2.88617631D+00 6.81933733D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.006750607 -0.003905369 0.001942316

2 6 -0.000423244 0.000288260 0.000555322

3 8 -0.006008648 0.005030303 -0.003115112

4 8 0.000423776 -0.001182316 0.001280208

5 6 0.000308475 -0.000582148 0.000558373

6 16 0.000398483 0.000019569 -0.000919175

7 6 0.000049535 -0.000297621 0.000658648

8 16 0.000857854 -0.000749354 -0.000210808

9 16 0.000354653 0.001662546 -0.000291140

10 6 -0.000672779 -0.000400046 -0.000165819

11 6 -0.000091424 -0.000109802 0.000085915

12 6 0.000046574 -0.000007987 -0.000120819

13 6 0.000299754 -0.000048141 -0.000003745

14 1 -0.000626681 0.000500931 0.000748385

15 1 -0.001065907 -0.000346382 -0.000716163

16 1 0.000175939 0.000178352 0.000005103

17 1 -0.000653728 0.000102873 0.000132019

18 1 -0.000132170 -0.000852735 -0.000290550

19 1 0.000104162 0.000567854 -0.000669057

20 1 -0.000218874 0.000338339 0.000781978

21 1 -0.000050754 -0.000301382 0.000499424

22 1 0.000066048 -0.000289591 -0.000648489

23 1 0.000044830 0.000379593 -0.000542865

24 1 0.000005988 0.000219928 0.000614360

25 1 0.000461798 0.000476914 -0.000053881

26 1 -0.000224127 -0.000423770 0.000465725

27 1 -0.000180141 -0.000268819 -0.000580151

-------------------------------------------------------------------

Cartesian Forces: Max 0.006750607 RMS 0.001386828

Leave Link 716 at Sat Aug 17 17:33:35 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.008409114 RMS 0.000984457

Search for a local minimum.

Step number 10 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .98446D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10

DE= 2.93D-04 DEPred=-2.11D-04 R=-1.39D+00

Trust test=-1.39D+00 RLast= 3.30D-01 DXMaxT set to 5.00D-02

ITU= -1 0 0 -1 0 0 -1 -1 0 0

Eigenvalues --- 0.00259 0.00330 0.00363 0.00397 0.00473

Eigenvalues --- 0.00480 0.00698 0.01040 0.01244 0.01325

Eigenvalues --- 0.02313 0.02782 0.03506 0.03630 0.04677

Eigenvalues --- 0.04829 0.04864 0.04948 0.05315 0.05440

Eigenvalues --- 0.05476 0.05563 0.05646 0.05875 0.08246

Eigenvalues --- 0.08343 0.08658 0.11249 0.12141 0.12218

Eigenvalues --- 0.13947 0.15759 0.15993 0.16000 0.16004

Eigenvalues --- 0.16040 0.16325 0.16400 0.18432 0.18986

Eigenvalues --- 0.19717 0.21904 0.21934 0.22146 0.23505

Eigenvalues --- 0.24368 0.24925 0.25044 0.25454 0.26657

Eigenvalues --- 0.26861 0.29101 0.29328 0.29507 0.29720

Eigenvalues --- 0.30274 0.31822 0.32935 0.33865 0.33872

Eigenvalues --- 0.33883 0.33900 0.34015 0.34034 0.34087

Eigenvalues --- 0.34177 0.34181 0.34447 0.34512 0.34526

Eigenvalues --- 0.34895 0.41318 0.52635 0.56777 1.86856

En-DIIS/RFO-DIIS IScMMF= 0 using points: 10 9 8

RFO step: Lambda=-1.73280561D-04.

NNeg= 0 NP= 3 Switch= 2.50D-03 Rises=T DC= 1.44D-06 SmlDif= 1.00D-05

RMS Error= 0.2144699826D-02 NUsed= 3 EDIIS=F

DidBck=T Rises=T RFO-DIIS coefs: 0.36745 0.73932 -0.10676

Iteration 1 RMS(Cart)= 0.09903511 RMS(Int)= 0.00244567

Iteration 2 RMS(Cart)= 0.00507756 RMS(Int)= 0.00008275

Iteration 3 RMS(Cart)= 0.00001447 RMS(Int)= 0.00008261

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00008261

ITry= 1 IFail=0 DXMaxC= 3.20D-01 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83846 0.00033 -0.00386 0.00484 0.00098 2.83944

R2 2.27821 0.00841 0.00816 -0.00096 0.00720 2.28541

R3 2.55110 0.00158 -0.00002 0.00256 0.00253 2.55363

R4 2.86525 0.00074 0.00265 -0.00032 0.00233 2.86759

R5 3.59002 0.00168 0.00142 0.00364 0.00505 3.59507

R6 2.05513 0.00079 0.00167 0.00059 0.00226 2.05738

R7 1.83402 0.00132 0.00198 0.00049 0.00247 1.83649

R8 2.05983 0.00024 0.00153 -0.00027 0.00126 2.06110

R9 2.06749 0.00053 0.00101 0.00051 0.00151 2.06900

R10 2.05815 0.00081 0.00135 0.00058 0.00194 2.06008

R11 3.32158 0.00085 0.00170 0.00067 0.00236 3.32394

R12 3.38310 0.00078 0.00372 -0.00166 0.00206 3.38516

R13 3.25134 0.00127 0.00092 0.00111 0.00204 3.25337

R14 3.47553 -0.00031 -0.00274 0.00260 -0.00014 3.47539

R15 2.87959 0.00058 0.00144 0.00046 0.00191 2.88149

R16 2.06194 0.00088 0.00158 0.00053 0.00211 2.06405

R17 2.05809 0.00080 0.00121 0.00077 0.00198 2.06007

R18 2.89203 0.00054 0.00121 0.00050 0.00170 2.89373

R19 2.07059 0.00060 0.00082 0.00069 0.00151 2.07210

R20 2.06925 0.00068 0.00114 0.00053 0.00167 2.07092

R21 2.88484 0.00047 0.00135 0.00028 0.00163 2.88647

R22 2.07011 0.00066 0.00103 0.00057 0.00161 2.07172

R23 2.06999 0.00063 0.00102 0.00055 0.00157 2.07156

R24 2.06599 0.00063 0.00090 0.00071 0.00161 2.06759

R25 2.06734 0.00065 0.00102 0.00062 0.00164 2.06899

R26 2.06726 0.00062 0.00095 0.00065 0.00160 2.06886

A1 2.18123 -0.00080 -0.00012 -0.00159 -0.00171 2.17952

A2 1.96962 0.00071 0.00228 0.00051 0.00279 1.97241

A3 2.13151 0.00012 -0.00183 0.00113 -0.00069 2.13082

A4 2.01850 -0.00049 -0.00164 0.00010 -0.00153 2.01697

A5 1.84222 -0.00074 0.00572 -0.00512 0.00060 1.84282

A6 1.87308 0.00001 -0.00049 -0.00248 -0.00298 1.87010

A7 1.94623 0.00113 0.00154 0.00269 0.00425 1.95048

A8 1.94061 0.00005 0.00133 -0.00154 -0.00022 1.94039

A9 1.83094 0.00002 -0.00693 0.00676 -0.00018 1.83076

A10 1.87602 0.00000 -0.00381 0.00503 0.00122 1.87724

A11 1.91470 -0.00003 -0.00067 0.00048 -0.00018 1.91452

A12 1.92978 -0.00063 -0.00147 -0.00116 -0.00263 1.92715

A13 1.95224 -0.00004 -0.00163 0.00228 0.00065 1.95289

A14 1.88136 0.00031 0.00087 -0.00034 0.00053 1.88189

A15 1.89255 0.00022 0.00099 0.00029 0.00127 1.89382

A16 1.89141 0.00020 0.00206 -0.00163 0.00043 1.89183

A17 1.79023 0.00401 -0.00272 0.00706 0.00433 1.79456

A18 1.96672 -0.00010 -0.00102 0.00723 0.00568 1.97241

A19 2.14083 -0.00005 0.00206 0.00230 0.00384 2.14467

A20 2.14933 0.00067 0.00697 -0.00147 0.00496 2.15429

A21 1.79693 -0.00096 -0.00078 -0.00053 -0.00132 1.79561

A22 1.92451 0.00005 -0.00085 0.00146 0.00061 1.92512

A23 1.87650 0.00019 0.00272 -0.00193 0.00079 1.87729

A24 1.89684 -0.00034 -0.00272 0.00147 -0.00125 1.89559

A25 1.93889 -0.00015 -0.00048 0.00019 -0.00029 1.93860

A26 1.93815 0.00020 0.00105 -0.00110 -0.00004 1.93810

A27 1.88717 0.00003 0.00029 -0.00011 0.00017 1.88734

A28 1.95549 -0.00006 -0.00076 0.00033 -0.00043 1.95506

A29 1.91633 0.00000 -0.00028 0.00001 -0.00027 1.91606

A30 1.91510 0.00006 0.00033 0.00015 0.00048 1.91558

A31 1.90624 0.00001 0.00052 -0.00074 -0.00023 1.90601

A32 1.90991 -0.00005 -0.00132 0.00091 -0.00041 1.90950

A33 1.85820 0.00005 0.00163 -0.00071 0.00092 1.85913

A34 1.96592 -0.00001 -0.00047 0.00066 0.00020 1.96611

A35 1.90676 0.00006 -0.00038 0.00041 0.00003 1.90679

A36 1.90861 -0.00009 -0.00037 -0.00030 -0.00067 1.90794

A37 1.91254 -0.00005 0.00000 0.00009 0.00009 1.91263

A38 1.91347 0.00003 -0.00048 0.00003 -0.00045 1.91302

A39 1.85312 0.00006 0.00183 -0.00099 0.00083 1.85395

A40 1.94685 -0.00017 -0.00171 0.00101 -0.00070 1.94615

A41 1.94402 -0.00018 -0.00143 0.00046 -0.00097 1.94306

A42 1.94323 -0.00016 -0.00097 0.00032 -0.00065 1.94258

A43 1.87443 0.00024 0.00207 -0.00086 0.00121 1.87564

A44 1.87562 0.00018 0.00181 -0.00098 0.00083 1.87645

A45 1.87607 0.00013 0.00049 -0.00007 0.00043 1.87650

D1 2.59226 -0.00041 -0.02087 0.01273 -0.00813 2.58413

D2 -1.53073 0.00016 -0.01557 0.01236 -0.00320 -1.53393

D3 0.41526 -0.00014 -0.02107 0.01667 -0.00439 0.41087

D4 -0.59216 0.00023 -0.01032 0.01408 0.00376 -0.58841

D5 1.56803 0.00080 -0.00501 0.01370 0.00868 1.57672

D6 -2.76916 0.00050 -0.01051 0.01802 0.00750 -2.76167

D7 -3.10477 -0.00022 -0.00608 0.00240 -0.00369 -3.10846

D8 -0.00461 0.00037 0.00415 0.00362 0.00779 0.00317

D9 -3.12374 -0.00001 0.00450 -0.00555 -0.00105 -3.12479

D10 -1.05105 -0.00003 0.00426 -0.00638 -0.00212 -1.05317

D11 1.05862 -0.00024 0.00476 -0.00772 -0.00295 1.05567

D12 1.05469 0.00044 -0.00316 -0.00092 -0.00408 1.05061

D13 3.12738 0.00042 -0.00340 -0.00175 -0.00515 3.12223

D14 -1.04613 0.00021 -0.00289 -0.00309 -0.00598 -1.05212

D15 -0.98209 -0.00033 0.00367 -0.01007 -0.00641 -0.98850

D16 1.09060 -0.00035 0.00343 -0.01091 -0.00748 1.08312

D17 -3.08291 -0.00056 0.00393 -0.01224 -0.00831 -3.09123

D18 -3.06546 -0.00080 -0.11701 0.01484 -0.10216 3.11557

D19 -0.86030 -0.00121 -0.11405 0.01312 -0.10094 -0.96124

D20 1.24212 -0.00052 -0.11587 0.01687 -0.09901 1.14311

D21 1.84469 0.00055 -0.00247 0.04246 0.04007 1.88476

D22 -1.05926 -0.00182 -0.04474 0.00687 -0.03795 -1.09720

D23 2.57495 -0.00091 -0.02830 -0.01508 -0.04338 2.53157

D24 -0.80563 0.00135 0.01365 0.02131 0.03496 -0.77067

D25 -3.03013 0.00017 0.01130 -0.01599 -0.00469 -3.03483

D26 -0.91393 0.00014 0.01191 -0.01609 -0.00419 -0.91812

D27 1.12486 0.00010 0.01227 -0.01649 -0.00422 1.12064

D28 -3.11468 0.00016 -0.00965 0.00967 0.00002 -3.11466

D29 -0.99329 0.00014 -0.00970 0.00895 -0.00075 -0.99403

D30 1.04331 0.00023 -0.00769 0.00819 0.00050 1.04380

D31 1.08990 -0.00002 -0.01219 0.01101 -0.00118 1.08872

D32 -3.07190 -0.00004 -0.01224 0.01029 -0.00194 -3.07384

D33 -1.03530 0.00005 -0.01023 0.00953 -0.00070 -1.03600

D34 -1.01110 -0.00009 -0.01294 0.01176 -0.00117 -1.01227

D35 1.11029 -0.00011 -0.01299 0.01105 -0.00194 1.10835

D36 -3.13630 -0.00002 -0.01098 0.01028 -0.00069 -3.13700

D37 -3.11661 0.00001 -0.00681 0.00403 -0.00278 -3.11939

D38 -0.98693 -0.00001 -0.00740 0.00489 -0.00251 -0.98943

D39 1.03439 0.00004 -0.00563 0.00377 -0.00186 1.03252

D40 1.03940 0.00004 -0.00632 0.00432 -0.00200 1.03740

D41 -3.11410 0.00002 -0.00690 0.00518 -0.00173 -3.11583

D42 -1.09279 0.00007 -0.00513 0.00405 -0.00108 -1.09387

D43 -0.98844 0.00001 -0.00782 0.00508 -0.00274 -0.99119

D44 1.14124 -0.00002 -0.00841 0.00593 -0.00247 1.13877

D45 -3.12063 0.00004 -0.00664 0.00481 -0.00183 -3.12246

D46 -3.13778 0.00003 -0.00654 0.00843 0.00189 -3.13589

D47 -1.04358 0.00010 -0.00604 0.00833 0.00229 -1.04129

D48 1.05025 0.00003 -0.00703 0.00877 0.00174 1.05199

D49 1.01899 0.00000 -0.00574 0.00739 0.00165 1.02064

D50 3.11319 0.00007 -0.00523 0.00729 0.00205 3.11524

D51 -1.07617 0.00000 -0.00622 0.00773 0.00151 -1.07467

D52 -1.00833 -0.00006 -0.00767 0.00851 0.00085 -1.00749

D53 1.08587 0.00001 -0.00716 0.00841 0.00125 1.08712

D54 -3.10349 -0.00006 -0.00815 0.00886 0.00070 -3.10279

Item Value Threshold Converged?

Maximum Force 0.008409 0.000450 NO

RMS Force 0.000984 0.000300 NO

Maximum Displacement 0.319812 0.001800 NO

RMS Displacement 0.100407 0.001200 NO

Predicted change in Energy=-2.893093D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:33:35 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.121085 -0.389100 -0.207501

2 6 0 -2.847475 0.049549 0.458238

3 8 0 -4.923434 0.354421 -0.723280

4 8 0 -4.279350 -1.731114 -0.212723

5 6 0 -2.389717 -0.806589 1.624502

6 16 0 -1.542978 0.112346 -0.925085

7 6 0 -0.105040 0.671714 -0.080479

8 16 0 1.128152 -0.610794 0.127698

9 16 0 -0.008076 2.213224 0.679973

10 6 0 2.710740 0.313036 -0.027981

11 6 0 3.890002 -0.653617 -0.026100

12 6 0 5.232175 0.078062 -0.116049

13 6 0 6.422676 -0.878441 -0.146481

14 1 0 -2.984199 1.086280 0.761233

15 1 0 -5.105784 -1.927019 -0.685036

16 1 0 -1.471338 -0.394698 2.044644

17 1 0 -3.147149 -0.811618 2.415077

18 1 0 -2.200559 -1.836931 1.322778

19 1 0 2.670274 0.881375 -0.959841

20 1 0 2.783229 1.020598 0.798161

21 1 0 3.870652 -1.260838 0.886722

22 1 0 3.798510 -1.351141 -0.866367

23 1 0 5.242100 0.705870 -1.014739

24 1 0 5.330676 0.761018 0.735757

25 1 0 7.371301 -0.336415 -0.205007

26 1 0 6.455499 -1.502129 0.752772

27 1 0 6.372360 -1.548685 -1.010663

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.502566 0.000000

3 O 1.209387 2.408015 0.000000

4 O 1.351323 2.381431 2.241644 0.000000

5 C 2.555028 1.517461 3.644138 2.793000 0.000000

6 S 2.722684 1.902430 3.395116 3.375431 2.839332

7 C 4.155728 2.863259 4.871425 4.818291 3.211244

8 S 5.264598 4.043627 6.186881 5.532818 3.828076

9 S 4.947377 3.576708 5.439210 5.882048 3.960255

10 C 6.870156 5.585659 7.665883 7.285192 5.477127

11 C 8.017504 6.791364 8.898250 8.242216 6.494825

12 C 9.365365 8.100084 10.177500 9.682539 7.867996

13 C 10.555286 9.336089 11.427461 10.736144 8.988872

14 H 2.099453 1.088719 2.549515 3.250186 2.163699

15 H 1.887556 3.211519 2.289036 0.971829 3.737158

16 H 3.477549 2.146577 4.487710 3.842739 1.090685

17 H 2.829309 2.158850 3.790002 3.005442 1.094869

18 H 2.850682 2.173646 4.049991 2.586567 1.090148

19 H 6.950013 5.757468 7.615645 7.461940 5.927189

20 H 7.118157 5.723925 7.883606 7.646818 5.548047

21 H 8.113267 6.858130 9.084994 8.237261 6.320039

22 H 8.004974 6.919944 8.888291 8.113165 6.692916

23 H 9.461491 8.248736 10.175782 9.861040 8.215702

24 H 9.568087 8.213730 10.365369 9.973110 7.927908

25 H 11.492507 10.247548 12.325030 11.733836 9.942115

26 H 10.678252 9.436089 11.623494 10.780611 8.915242

27 H 10.587827 9.471926 11.458593 10.683113 9.179804

6 7 8 9 10

6 S 0.000000

7 C 1.758953 0.000000

8 S 2.960780 1.791348 0.000000

9 S 3.057095 1.721611 3.093720 0.000000

10 C 4.351918 2.839018 1.839098 3.391737 0.000000

11 C 5.559869 4.209492 2.766460 4.890023 1.524821

12 C 6.823373 5.370247 4.168566 5.714263 2.533891

13 C 8.064709 6.709577 5.308370 7.183035 3.900273

14 H 2.422671 3.028184 4.493646 3.183381 5.801128

15 H 4.112204 5.668010 6.423001 6.707570 8.157672

16 H 3.013555 2.742289 3.237086 3.287053 4.720851

17 H 3.818869 4.205057 4.852900 4.691912 6.445793

18 H 3.047127 3.557194 3.743254 4.650155 5.528812

19 H 4.283002 2.918836 2.405712 3.411213 1.092250

20 H 4.744531 3.039051 2.418727 3.037715 1.090142

21 H 5.871599 4.525082 2.918901 5.211180 2.158508

22 H 5.538658 4.466236 2.943992 5.439298 2.157689

23 H 6.811577 5.428252 4.468034 5.719136 2.745140

24 H 7.101147 5.497384 4.462377 5.533018 2.765510

25 H 8.954567 7.545032 6.258026 7.857421 4.708923

26 H 8.330508 6.961363 5.437446 7.455666 4.234102

27 H 8.088196 6.910291 5.447680 7.597380 4.223639

11 12 13 14 15

11 C 0.000000

12 C 1.531298 0.000000

13 C 2.545482 1.527454 0.000000

14 H 7.134547 8.324357 9.652635 0.000000

15 H 9.109331 10.545970 11.588569 3.958887 0.000000

16 H 5.753171 7.058979 8.206735 2.475719 4.796703

17 H 7.450222 8.798364 9.906947 2.522651 3.832893

18 H 6.349381 7.809159 8.799864 3.078081 3.532671

19 H 2.171591 2.814362 4.223627 5.914148 8.272223

20 H 2.169642 2.778757 4.212395 5.767921 8.551307

21 H 1.096511 2.156837 2.779669 7.246633 9.137320

22 H 1.095883 2.158934 2.761871 7.388859 8.924739

23 H 2.157262 1.096305 2.158164 8.424415 10.682673

24 H 2.158045 1.096223 2.158387 8.321273 10.870321

25 H 3.500296 2.180726 1.094124 10.497336 12.587220

26 H 2.812186 2.179076 1.094861 9.788147 11.658091

27 H 2.816490 2.178684 1.094792 9.880680 11.488992

16 17 18 19 20

16 H 0.000000

17 H 1.766179 0.000000

18 H 1.769997 1.772122 0.000000

19 H 5.273352 6.935324 6.026986 0.000000

20 H 4.653829 6.414111 5.768782 1.767120 0.000000

21 H 5.534243 7.196333 6.114052 3.072422 2.528890

22 H 6.095906 7.700724 6.404466 2.503154 3.070276

23 H 7.459311 9.189445 8.205059 2.578391 3.071108

24 H 7.022553 8.784465 7.988331 3.157099 2.561398

25 H 9.124505 10.850275 9.808475 4.914513 4.888582

26 H 8.107409 9.769899 8.681264 4.789787 4.455533

27 H 8.496480 10.143964 8.889487 4.428681 4.770211

21 22 23 24 25

21 H 0.000000

22 H 1.756895 0.000000

23 H 3.060124 2.517391 0.000000

24 H 2.498472 3.061952 1.753603 0.000000

25 H 3.781663 3.772520 2.505099 2.500709 0.000000

26 H 2.599537 3.115124 3.077611 2.527321 1.764914

27 H 3.153009 2.585449 2.522008 3.077307 1.765380

26 27

26 H 0.000000

27 H 1.766007 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 6.42D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.134388 -0.405097 -0.162277

2 6 0 -2.855621 0.121325 0.425376

3 8 0 -4.937076 0.257884 -0.777717

4 8 0 -4.297214 -1.732636 0.030601

5 6 0 -2.394280 -0.556019 1.702505

6 16 0 -1.558632 -0.025283 -0.958663

7 6 0 -0.114137 0.646149 -0.212653

8 16 0 1.115852 -0.596959 0.175594

9 16 0 -0.007736 2.282262 0.312472

10 6 0 2.700663 0.287369 -0.122097

11 6 0 3.876643 -0.673409 0.015942

12 6 0 5.220761 0.031516 -0.187288

13 6 0 6.407835 -0.924019 -0.082759

14 1 0 -2.987153 1.191887 0.573381

15 1 0 -5.126920 -1.992387 -0.403647

16 1 0 -1.472192 -0.090679 2.052942

17 1 0 -3.147317 -0.441657 2.489013

18 1 0 -2.210286 -1.620293 1.554556

19 1 0 2.656937 0.712753 -1.127158

20 1 0 2.780137 1.108352 0.590700

21 1 0 3.860319 -1.139802 1.008185

22 1 0 3.778123 -1.486460 -0.712208

23 1 0 5.227810 0.520387 -1.168532

24 1 0 5.326305 0.831823 0.554381

25 1 0 7.357946 -0.400430 -0.225063

26 1 0 6.443550 -1.408910 0.898222

27 1 0 6.350448 -1.713772 -0.838779

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3464241 0.1906828 0.1790087

Leave Link 202 at Sat Aug 17 17:33:35 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1100.2327037321 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0547723222 Hartrees.

Nuclear repulsion after empirical dispersion term = 1100.1779314098 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2308

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.27D-10

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 82

GePol: Fraction of low-weight points (<1% of avg) = 3.55%

GePol: Cavity surface area = 309.845 Ang\*\*2

GePol: Cavity volume = 320.381 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057010615 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1100.1722303483 Hartrees.

Leave Link 301 at Sat Aug 17 17:33:35 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:33:35 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:33:35 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999874 -0.015650 0.001433 0.002065 Ang= -1.82 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.62961069335

Leave Link 401 at Sat Aug 17 17:33:36 2019, MaxMem= 1342177280 cpu: 7.5

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 15980592.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.77D-15 for 383.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.42D-15 for 2296 1769.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.77D-15 for 2294.

Iteration 1 A^-1\*A deviation from orthogonality is 1.76D-11 for 896 892.

E= -1658.65974425657

DIIS: error= 4.38D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.65974425657 IErMin= 1 ErrMin= 4.38D-03

ErrMax= 4.38D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.21D-02 BMatP= 4.21D-02

IDIUse=3 WtCom= 9.56D-01 WtEn= 4.38D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.428 Goal= None Shift= 0.000

Gap= 0.484 Goal= None Shift= 0.000

GapD= 0.428 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=4.59D-04 MaxDP=1.12D-02 OVMax= 2.66D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.59D-04 CP: 9.99D-01

E= -1658.67659505896 Delta-E= -0.016850802392 Rises=F Damp=F

DIIS: error= 6.02D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67659505896 IErMin= 2 ErrMin= 6.02D-04

ErrMax= 6.02D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.45D-04 BMatP= 4.21D-02

IDIUse=3 WtCom= 9.94D-01 WtEn= 6.02D-03

Coeff-Com: -0.562D-01 0.106D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.559D-01 0.106D+01

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=7.58D-05 MaxDP=2.77D-03 DE=-1.69D-02 OVMax= 4.79D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 7.17D-05 CP: 9.99D-01 1.05D+00

E= -1658.67668842456 Delta-E= -0.000093365603 Rises=F Damp=F

DIIS: error= 1.05D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67668842456 IErMin= 2 ErrMin= 6.02D-04

ErrMax= 1.05D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.32D-04 BMatP= 6.45D-04

IDIUse=3 WtCom= 9.89D-01 WtEn= 1.05D-02

Coeff-Com: -0.370D-01 0.562D+00 0.475D+00

Coeff-En: 0.000D+00 0.223D+00 0.777D+00

Coeff: -0.366D-01 0.558D+00 0.478D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=4.10D-05 MaxDP=1.62D-03 DE=-9.34D-05 OVMax= 4.54D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.82D-05 CP: 9.99D-01 1.07D+00 6.10D-01

E= -1658.67678635484 Delta-E= -0.000097930273 Rises=F Damp=F

DIIS: error= 5.23D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67678635484 IErMin= 4 ErrMin= 5.23D-04

ErrMax= 5.23D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.40D-04 BMatP= 6.32D-04

IDIUse=3 WtCom= 9.95D-01 WtEn= 5.23D-03

Coeff-Com: -0.125D-01 0.173D+00 0.321D+00 0.519D+00

Coeff-En: 0.000D+00 0.000D+00 0.188D+00 0.812D+00

Coeff: -0.124D-01 0.172D+00 0.320D+00 0.521D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=1.54D-05 MaxDP=5.83D-04 DE=-9.79D-05 OVMax= 1.64D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.13D-05 CP: 9.99D-01 1.08D+00 6.72D-01 6.85D-01

E= -1658.67681101035 Delta-E= -0.000024655516 Rises=F Damp=F

DIIS: error= 6.61D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67681101035 IErMin= 5 ErrMin= 6.61D-05

ErrMax= 6.61D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.27D-06 BMatP= 1.40D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.339D-02 0.412D-01 0.121D+00 0.254D+00 0.587D+00

Coeff: -0.339D-02 0.412D-01 0.121D+00 0.254D+00 0.587D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=4.63D-06 MaxDP=2.13D-04 DE=-2.47D-05 OVMax= 3.32D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.68D-06 CP: 9.99D-01 1.08D+00 6.96D-01 7.37D-01 8.60D-01

E= -1658.67681217253 Delta-E= -0.000001162180 Rises=F Damp=F

DIIS: error= 2.79D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67681217253 IErMin= 6 ErrMin= 2.79D-05

ErrMax= 2.79D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.51D-07 BMatP= 5.27D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.588D-03-0.124D-01 0.517D-02 0.409D-01 0.306D+00 0.660D+00

Coeff: 0.588D-03-0.124D-01 0.517D-02 0.409D-01 0.306D+00 0.660D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=2.20D-06 MaxDP=7.91D-05 DE=-1.16D-06 OVMax= 2.03D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.53D-06 CP: 9.99D-01 1.08D+00 7.07D-01 7.65D-01 9.43D-01

CP: 8.50D-01

E= -1658.67681240958 Delta-E= -0.000000237055 Rises=F Damp=F

DIIS: error= 7.68D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67681240958 IErMin= 7 ErrMin= 7.68D-06

ErrMax= 7.68D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.68D-08 BMatP= 8.51D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.657D-03-0.105D-01-0.129D-01-0.136D-01 0.556D-01 0.287D+00

Coeff-Com: 0.694D+00

Coeff: 0.657D-03-0.105D-01-0.129D-01-0.136D-01 0.556D-01 0.287D+00

Coeff: 0.694D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=9.15D-07 MaxDP=4.44D-05 DE=-2.37D-07 OVMax= 9.31D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 6.11D-07 CP: 9.99D-01 1.08D+00 7.10D-01 7.75D-01 9.73D-01

CP: 9.67D-01 1.14D+00

E= -1658.67681243903 Delta-E= -0.000000029445 Rises=F Damp=F

DIIS: error= 3.73D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67681243903 IErMin= 8 ErrMin= 3.73D-06

ErrMax= 3.73D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.33D-08 BMatP= 9.68D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.196D-03-0.237D-02-0.726D-02-0.149D-01-0.365D-01 0.732D-02

Coeff-Com: 0.351D+00 0.703D+00

Coeff: 0.196D-03-0.237D-02-0.726D-02-0.149D-01-0.365D-01 0.732D-02

Coeff: 0.351D+00 0.703D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=4.85D-07 MaxDP=2.15D-05 DE=-2.94D-08 OVMax= 4.71D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.29D-07 CP: 9.99D-01 1.08D+00 7.11D-01 7.80D-01 9.86D-01

CP: 1.03D+00 1.33D+00 9.02D-01

E= -1658.67681244647 Delta-E= -0.000000007438 Rises=F Damp=F

DIIS: error= 1.03D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67681244647 IErMin= 9 ErrMin= 1.03D-06

ErrMax= 1.03D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.36D-09 BMatP= 2.33D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.934D-05 0.570D-03-0.153D-02-0.542D-02-0.265D-01-0.427D-01

Coeff-Com: 0.484D-01 0.322D+00 0.705D+00

Coeff: -0.934D-05 0.570D-03-0.153D-02-0.542D-02-0.265D-01-0.427D-01

Coeff: 0.484D-01 0.322D+00 0.705D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=2.41D-07 MaxDP=1.17D-05 DE=-7.44D-09 OVMax= 2.90D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.16D-07 CP: 9.99D-01 1.08D+00 7.12D-01 7.80D-01 9.91D-01

CP: 1.04D+00 1.42D+00 1.10D+00 7.59D-01

E= -1658.67681244734 Delta-E= -0.000000000874 Rises=F Damp=F

DIIS: error= 8.61D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67681244734 IErMin=10 ErrMin= 8.61D-07

ErrMax= 8.61D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.60D-09 BMatP= 3.36D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.330D-04 0.709D-03 0.206D-04-0.148D-02-0.117D-01-0.290D-01

Coeff-Com: -0.247D-01 0.101D+00 0.481D+00 0.484D+00

Coeff: -0.330D-04 0.709D-03 0.206D-04-0.148D-02-0.117D-01-0.290D-01

Coeff: -0.247D-01 0.101D+00 0.481D+00 0.484D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=8.60D-08 MaxDP=4.13D-06 DE=-8.74D-10 OVMax= 8.48D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 3.99D-08 CP: 9.99D-01 1.08D+00 7.12D-01 7.81D-01 9.91D-01

CP: 1.05D+00 1.44D+00 1.10D+00 9.17D-01 6.33D-01

E= -1658.67681244778 Delta-E= -0.000000000433 Rises=F Damp=F

DIIS: error= 1.88D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67681244778 IErMin=11 ErrMin= 1.88D-07

ErrMax= 1.88D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.79D-11 BMatP= 1.60D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.129D-04 0.241D-03 0.142D-03-0.163D-03-0.224D-02-0.791D-02

Coeff-Com: -0.168D-01 0.946D-02 0.147D+00 0.225D+00 0.645D+00

Coeff: -0.129D-04 0.241D-03 0.142D-03-0.163D-03-0.224D-02-0.791D-02

Coeff: -0.168D-01 0.946D-02 0.147D+00 0.225D+00 0.645D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=2.51D-08 MaxDP=1.03D-06 DE=-4.33D-10 OVMax= 3.39D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.46D-08 CP: 9.99D-01 1.08D+00 7.12D-01 7.81D-01 9.91D-01

CP: 1.05D+00 1.45D+00 1.12D+00 9.34D-01 7.37D-01

CP: 9.85D-01

E= -1658.67681244780 Delta-E= -0.000000000023 Rises=F Damp=F

DIIS: error= 7.70D-08 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.67681244780 IErMin=12 ErrMin= 7.70D-08

ErrMax= 7.70D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.28D-11 BMatP= 6.79D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.418D-06-0.335D-04 0.642D-04 0.229D-03 0.154D-02 0.258D-02

Coeff-Com: -0.367D-02-0.189D-01-0.300D-01 0.136D-01 0.324D+00 0.711D+00

Coeff: 0.418D-06-0.335D-04 0.642D-04 0.229D-03 0.154D-02 0.258D-02

Coeff: -0.367D-02-0.189D-01-0.300D-01 0.136D-01 0.324D+00 0.711D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=1.14D-08 MaxDP=4.81D-07 DE=-2.32D-11 OVMax= 1.30D-06

Cycle 13 Pass 1 IDiag 1:

RMSU= 5.68D-09 CP: 9.99D-01 1.08D+00 7.12D-01 7.81D-01 9.91D-01

CP: 1.05D+00 1.45D+00 1.12D+00 9.49D-01 7.73D-01

CP: 1.13D+00 9.89D-01

E= -1658.67681244778 Delta-E= 0.000000000023 Rises=F Damp=F

DIIS: error= 2.62D-08 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=12 EnMin= -1658.67681244780 IErMin=13 ErrMin= 2.62D-08

ErrMax= 2.62D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.86D-13 BMatP= 1.28D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.183D-05-0.406D-04-0.431D-06 0.902D-04 0.729D-03 0.188D-02

Coeff-Com: 0.125D-02-0.655D-02-0.285D-01-0.259D-01-0.823D-02 0.182D+00

Coeff-Com: 0.883D+00

Coeff: 0.183D-05-0.406D-04-0.431D-06 0.902D-04 0.729D-03 0.188D-02

Coeff: 0.125D-02-0.655D-02-0.285D-01-0.259D-01-0.823D-02 0.182D+00

Coeff: 0.883D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=5.55D-09 MaxDP=3.04D-07 DE= 2.27D-11 OVMax= 7.25D-07

Error on total polarization charges = 0.04178

SCF Done: E(UB3LYP) = -1658.67681245 A.U. after 13 cycles

NFock= 13 Conv=0.56D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7553 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655234628989D+03 PE=-6.143101842604D+03 EE= 1.729018170819D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.58

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7553, after 0.7500

Leave Link 502 at Sat Aug 17 17:34:03 2019, MaxMem= 1342177280 cpu: 312.8

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 340

Leave Link 701 at Sat Aug 17 17:34:04 2019, MaxMem= 1342177280 cpu: 10.2

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:34:04 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:34:07 2019, MaxMem= 1342177280 cpu: 35.9

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.33698710D+00-2.88550531D+00 5.65952753D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.001432171 -0.001227995 0.000879997

2 6 0.000039700 -0.000015324 0.000021966

3 8 -0.001153626 0.001207030 -0.001047746

4 8 0.000206083 -0.000169113 0.000194089

5 6 0.000053995 -0.000150010 0.000005146

6 16 0.000342443 0.000007912 0.000259300

7 6 -0.000067970 0.000034237 -0.000629059

8 16 -0.000484732 -0.000069413 0.000472286

9 16 -0.000310099 0.000055657 0.000367109

10 6 0.000018324 0.000000706 -0.000187612

11 6 -0.000089978 -0.000210477 0.000030164

12 6 -0.000018445 0.000116741 -0.000016432

13 6 0.000136170 -0.000137206 -0.000071770

14 1 -0.000043713 0.000035402 0.000172536

15 1 -0.000177227 0.000265984 -0.000095395

16 1 0.000322357 0.000198736 -0.000097632

17 1 -0.000108081 -0.000050447 0.000018785

18 1 0.000122762 -0.000055427 -0.000194400

19 1 0.000080822 0.000144394 -0.000049268

20 1 -0.000159869 -0.000069978 0.000123040

21 1 -0.000005872 -0.000024072 0.000049455

22 1 0.000036825 0.000011558 -0.000147198

23 1 -0.000013811 0.000044563 -0.000075124

24 1 -0.000022437 -0.000035982 0.000130533

25 1 0.000001945 0.000124230 -0.000012609

26 1 -0.000052122 -0.000056609 0.000018235

27 1 -0.000085615 0.000024903 -0.000118396

-------------------------------------------------------------------

Cartesian Forces: Max 0.001432171 RMS 0.000357007

Leave Link 716 at Sat Aug 17 17:34:07 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.001946839 RMS 0.000337977

Search for a local minimum.

Step number 11 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .33798D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 3 4 5 6

2 8 9 10 11

DE= -2.80D-04 DEPred=-2.89D-04 R= 9.67D-01

TightC=F SS= 1.41D+00 RLast= 1.94D-01 DXNew= 8.4090D-02 5.8173D-01

Trust test= 9.67D-01 RLast= 1.94D-01 DXMaxT set to 8.41D-02

ITU= 1 -1 0 0 -1 0 0 -1 -1 0 0

Eigenvalues --- 0.00270 0.00312 0.00342 0.00383 0.00426

Eigenvalues --- 0.00494 0.00557 0.00886 0.01112 0.01834

Eigenvalues --- 0.02317 0.02741 0.03508 0.03610 0.04632

Eigenvalues --- 0.04773 0.04843 0.04956 0.05005 0.05445

Eigenvalues --- 0.05470 0.05596 0.05639 0.05838 0.08240

Eigenvalues --- 0.08342 0.08634 0.11271 0.12141 0.12210

Eigenvalues --- 0.13849 0.15689 0.15998 0.16000 0.16024

Eigenvalues --- 0.16052 0.16224 0.16703 0.17765 0.18894

Eigenvalues --- 0.19838 0.21915 0.21936 0.22150 0.23522

Eigenvalues --- 0.24739 0.25056 0.25296 0.25471 0.26540

Eigenvalues --- 0.27992 0.28710 0.29160 0.29477 0.29762

Eigenvalues --- 0.30228 0.31968 0.33634 0.33848 0.33877

Eigenvalues --- 0.33881 0.33903 0.33943 0.34027 0.34040

Eigenvalues --- 0.34096 0.34222 0.34369 0.34520 0.34599

Eigenvalues --- 0.34940 0.36456 0.52645 0.56441 1.07806

En-DIIS/RFO-DIIS IScMMF= 0 using points: 11 10 9 8

RFO step: Lambda=-2.83115262D-05.

NNeg= 0 NP= 4 Switch= 2.50D-03 Rises=F DC= 1.44D-06 SmlDif= 1.00D-05

RMS Error= 0.9463343161D-03 NUsed= 4 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.54901 0.32280 1.16946 -1.04128

Iteration 1 RMS(Cart)= 0.02609853 RMS(Int)= 0.00027235

Iteration 2 RMS(Cart)= 0.00079041 RMS(Int)= 0.00002879

Iteration 3 RMS(Cart)= 0.00000044 RMS(Int)= 0.00002879

ITry= 1 IFail=0 DXMaxC= 1.08D-01 DCOld= 1.00D+10 DXMaxT= 8.41D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83944 -0.00024 -0.00148 0.00082 -0.00066 2.83878

R2 2.28541 0.00195 0.00176 0.00021 0.00196 2.28737

R3 2.55363 -0.00006 -0.00043 0.00043 0.00000 2.55363

R4 2.86759 -0.00011 0.00046 -0.00031 0.00015 2.86774

R5 3.59507 -0.00057 -0.00094 0.00159 0.00065 3.59572

R6 2.05738 0.00009 0.00012 0.00039 0.00051 2.05789

R7 1.83649 0.00013 0.00025 0.00023 0.00048 1.83697

R8 2.06110 0.00032 0.00034 0.00015 0.00049 2.06159

R9 2.06900 0.00010 0.00009 0.00022 0.00030 2.06931

R10 2.06008 0.00009 0.00008 0.00039 0.00047 2.06055

R11 3.32394 -0.00094 0.00008 -0.00122 -0.00114 3.32280

R12 3.38516 -0.00028 0.00084 -0.00128 -0.00044 3.38471

R13 3.25337 0.00017 -0.00011 0.00051 0.00040 3.25377

R14 3.47539 -0.00019 -0.00084 0.00044 -0.00040 3.47499

R15 2.88149 0.00004 0.00022 -0.00005 0.00017 2.88166

R16 2.06405 0.00012 0.00017 0.00028 0.00045 2.06451

R17 2.06007 0.00002 0.00010 0.00021 0.00030 2.06037

R18 2.89373 -0.00002 0.00011 0.00012 0.00023 2.89397

R19 2.07210 0.00007 0.00002 0.00030 0.00032 2.07242

R20 2.07092 0.00009 0.00009 0.00026 0.00035 2.07127

R21 2.88647 0.00005 0.00026 -0.00009 0.00018 2.88665

R22 2.07172 0.00009 0.00006 0.00030 0.00036 2.07208

R23 2.07156 0.00007 0.00007 0.00023 0.00030 2.07186

R24 2.06759 0.00006 0.00002 0.00026 0.00028 2.06788

R25 2.06899 0.00007 0.00007 0.00023 0.00030 2.06928

R26 2.06886 0.00007 0.00005 0.00023 0.00028 2.06914

A1 2.17952 -0.00008 0.00052 -0.00143 -0.00091 2.17861

A2 1.97241 0.00016 0.00032 0.00060 0.00093 1.97334

A3 2.13082 -0.00007 -0.00084 0.00078 -0.00005 2.13078

A4 2.01697 0.00053 -0.00008 -0.00023 -0.00031 2.01665

A5 1.84282 -0.00004 0.00226 -0.00335 -0.00110 1.84172

A6 1.87010 -0.00010 0.00124 -0.00247 -0.00123 1.86887

A7 1.95048 -0.00053 -0.00147 0.00258 0.00111 1.95159

A8 1.94039 -0.00009 0.00028 0.00053 0.00081 1.94121

A9 1.83076 0.00021 -0.00231 0.00296 0.00066 1.83141

A10 1.87724 -0.00049 -0.00129 -0.00086 -0.00215 1.87509

A11 1.91452 -0.00034 -0.00088 0.00096 0.00008 1.91460

A12 1.92715 0.00004 0.00031 -0.00116 -0.00085 1.92630

A13 1.95289 -0.00011 -0.00076 0.00014 -0.00061 1.95228

A14 1.88189 0.00019 0.00045 0.00010 0.00055 1.88243

A15 1.89382 0.00013 -0.00005 0.00055 0.00050 1.89433

A16 1.89183 0.00011 0.00097 -0.00058 0.00040 1.89223

A17 1.79456 -0.00182 -0.00291 0.00241 -0.00049 1.79407

A18 1.97241 -0.00114 -0.00325 0.00149 -0.00157 1.97083

A19 2.14467 0.00020 -0.00099 -0.00083 -0.00163 2.14303

A20 2.15429 0.00077 0.00061 -0.00132 -0.00053 2.15377

A21 1.79561 0.00028 0.00024 -0.00097 -0.00073 1.79488

A22 1.92512 -0.00022 -0.00048 0.00019 -0.00029 1.92483

A23 1.87729 0.00020 0.00099 -0.00043 0.00056 1.87785

A24 1.89559 -0.00011 -0.00062 -0.00035 -0.00097 1.89462

A25 1.93860 -0.00011 -0.00014 0.00001 -0.00013 1.93848

A26 1.93810 0.00026 0.00025 0.00033 0.00058 1.93869

A27 1.88734 -0.00002 0.00002 0.00021 0.00023 1.88757

A28 1.95506 -0.00011 -0.00009 -0.00054 -0.00062 1.95444

A29 1.91606 0.00006 -0.00008 0.00041 0.00033 1.91639

A30 1.91558 0.00001 -0.00003 -0.00006 -0.00009 1.91549

A31 1.90601 0.00004 0.00015 0.00026 0.00040 1.90641

A32 1.90950 0.00000 -0.00045 0.00007 -0.00038 1.90912

A33 1.85913 0.00001 0.00053 -0.00012 0.00041 1.85954

A34 1.96611 -0.00002 -0.00021 0.00010 -0.00011 1.96600

A35 1.90679 0.00001 -0.00029 0.00033 0.00005 1.90684

A36 1.90794 -0.00004 0.00000 -0.00023 -0.00023 1.90771

A37 1.91263 -0.00003 -0.00007 -0.00014 -0.00020 1.91242

A38 1.91302 0.00005 -0.00003 0.00016 0.00013 1.91315

A39 1.85395 0.00003 0.00064 -0.00024 0.00040 1.85436

A40 1.94615 -0.00011 -0.00045 -0.00005 -0.00050 1.94564

A41 1.94306 -0.00002 -0.00037 0.00020 -0.00017 1.94288

A42 1.94258 -0.00010 -0.00033 -0.00004 -0.00037 1.94221

A43 1.87564 0.00008 0.00048 0.00012 0.00060 1.87625

A44 1.87645 0.00010 0.00057 -0.00020 0.00037 1.87682

A45 1.87650 0.00006 0.00018 -0.00003 0.00015 1.87664

D1 2.58413 0.00034 -0.00478 0.01226 0.00748 2.59161

D2 -1.53393 -0.00003 -0.00499 0.01286 0.00787 -1.52606

D3 0.41087 0.00016 -0.00608 0.01369 0.00761 0.41848

D4 -0.58841 0.00029 -0.00384 0.01042 0.00659 -0.58182

D5 1.57672 -0.00007 -0.00405 0.01103 0.00698 1.58370

D6 -2.76167 0.00012 -0.00513 0.01185 0.00672 -2.75495

D7 -3.10846 -0.00002 -0.00144 0.00150 0.00005 -3.10841

D8 0.00317 -0.00006 -0.00051 -0.00032 -0.00083 0.00234

D9 -3.12479 -0.00014 0.00264 -0.00412 -0.00148 -3.12626

D10 -1.05317 -0.00009 0.00285 -0.00412 -0.00127 -1.05444

D11 1.05567 0.00000 0.00379 -0.00555 -0.00177 1.05391

D12 1.05061 -0.00006 0.00085 -0.00151 -0.00066 1.04995

D13 3.12223 -0.00002 0.00105 -0.00150 -0.00045 3.12178

D14 -1.05212 0.00008 0.00199 -0.00294 -0.00095 -1.05306

D15 -0.98850 0.00006 0.00448 -0.00719 -0.00271 -0.99121

D16 1.08312 0.00011 0.00468 -0.00719 -0.00251 1.08061

D17 -3.09123 0.00020 0.00562 -0.00862 -0.00300 -3.09423

D18 3.11557 0.00016 -0.02680 -0.00331 -0.03010 3.08546

D19 -0.96124 0.00045 -0.02625 -0.00431 -0.03055 -0.99179

D20 1.14311 0.00019 -0.02811 -0.00043 -0.02855 1.11456

D21 1.88476 -0.00080 -0.02798 0.00529 -0.02269 1.86207

D22 -1.09720 0.00026 -0.00927 0.00987 0.00061 -1.09660

D23 2.53157 0.00036 0.01685 -0.03387 -0.01699 2.51458

D24 -0.77067 -0.00077 -0.00212 -0.03842 -0.04057 -0.81124

D25 -3.03483 0.00027 0.00150 0.02239 0.02388 -3.01094

D26 -0.91812 0.00013 0.00166 0.02225 0.02391 -0.89421

D27 1.12064 0.00016 0.00189 0.02208 0.02397 1.14461

D28 -3.11466 0.00002 -0.00307 0.00165 -0.00141 -3.11607

D29 -0.99403 0.00004 -0.00299 0.00191 -0.00109 -0.99512

D30 1.04380 0.00010 -0.00242 0.00197 -0.00045 1.04335

D31 1.08872 -0.00001 -0.00389 0.00205 -0.00184 1.08688

D32 -3.07384 0.00000 -0.00382 0.00231 -0.00151 -3.07535

D33 -1.03600 0.00006 -0.00325 0.00237 -0.00088 -1.03688

D34 -1.01227 -0.00009 -0.00400 0.00156 -0.00244 -1.01471

D35 1.10835 -0.00007 -0.00392 0.00181 -0.00211 1.10624

D36 -3.13700 -0.00001 -0.00335 0.00187 -0.00148 -3.13847

D37 -3.11939 0.00009 -0.00176 0.00553 0.00376 -3.11563

D38 -0.98943 0.00004 -0.00220 0.00566 0.00346 -0.98597

D39 1.03252 0.00007 -0.00159 0.00543 0.00384 1.03636

D40 1.03740 0.00006 -0.00171 0.00518 0.00348 1.04088

D41 -3.11583 0.00001 -0.00214 0.00531 0.00317 -3.11265

D42 -1.09387 0.00003 -0.00153 0.00508 0.00355 -1.09032

D43 -0.99119 0.00003 -0.00217 0.00514 0.00297 -0.98822

D44 1.13877 -0.00002 -0.00260 0.00527 0.00267 1.14144

D45 -3.12246 0.00000 -0.00199 0.00504 0.00305 -3.11941

D46 -3.13589 0.00000 -0.00365 0.00515 0.00150 -3.13439

D47 -1.04129 0.00001 -0.00360 0.00541 0.00181 -1.03948

D48 1.05199 0.00001 -0.00384 0.00547 0.00163 1.05362

D49 1.02064 0.00002 -0.00309 0.00475 0.00166 1.02230

D50 3.11524 0.00004 -0.00304 0.00501 0.00197 3.11721

D51 -1.07467 0.00003 -0.00329 0.00507 0.00179 -1.07288

D52 -1.00749 -0.00003 -0.00381 0.00503 0.00122 -1.00627

D53 1.08712 -0.00001 -0.00376 0.00528 0.00153 1.08865

D54 -3.10279 -0.00002 -0.00400 0.00535 0.00134 -3.10145

Item Value Threshold Converged?

Maximum Force 0.001947 0.000450 NO

RMS Force 0.000338 0.000300 NO

Maximum Displacement 0.107503 0.001800 NO

RMS Displacement 0.026092 0.001200 NO

Predicted change in Energy=-1.553437D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:34:07 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.111875 -0.382998 -0.214430

2 6 0 -2.837077 0.038024 0.459576

3 8 0 -4.901304 0.373108 -0.734272

4 8 0 -4.288151 -1.722742 -0.224067

5 6 0 -2.392730 -0.831774 1.621014

6 16 0 -1.527799 0.098851 -0.919785

7 6 0 -0.100992 0.686317 -0.076635

8 16 0 1.129331 -0.588891 0.184586

9 16 0 -0.029099 2.238834 0.664440

10 6 0 2.712998 0.324937 -0.011426

11 6 0 3.888393 -0.646525 -0.003625

12 6 0 5.231745 0.078052 -0.128710

13 6 0 6.418121 -0.883717 -0.158957

14 1 0 -2.966291 1.073894 0.769693

15 1 0 -5.114778 -1.904311 -0.702259

16 1 0 -1.471077 -0.433150 2.047411

17 1 0 -3.153586 -0.833880 2.408532

18 1 0 -2.214328 -1.862023 1.311625

19 1 0 2.663133 0.873446 -0.954924

20 1 0 2.797899 1.049687 0.798692

21 1 0 3.879341 -1.233192 0.922896

22 1 0 3.782948 -1.362088 -0.827160

23 1 0 5.230064 0.688085 -1.039843

24 1 0 5.345835 0.777039 0.708221

25 1 0 7.367685 -0.346143 -0.241288

26 1 0 6.461451 -1.491186 0.751079

27 1 0 6.352302 -1.569291 -1.010162

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.502217 0.000000

3 O 1.210425 2.408026 0.000000

4 O 1.351325 2.381865 2.242510 0.000000

5 C 2.554549 1.517541 3.645827 2.791195 0.000000

6 S 2.721609 1.902773 3.389715 3.379610 2.840744

7 C 4.153265 2.862511 4.855263 4.832970 3.230895

8 S 5.260404 4.025051 6.175622 5.549930 3.811461

9 S 4.931073 3.573552 5.401454 5.884135 3.991293

10 C 6.864494 5.577409 7.648687 7.297553 5.483730

11 C 8.007383 6.776069 8.878754 8.250013 6.490476

12 C 9.355381 8.090338 10.155415 9.689188 7.875401

13 C 10.542041 9.321528 11.403507 10.739295 8.988998

14 H 2.098427 1.088988 2.548977 3.249006 2.164553

15 H 1.886315 3.210989 2.287626 0.972084 3.735971

16 H 3.477392 2.146900 4.489350 3.841688 1.090944

17 H 2.828700 2.158431 3.793225 3.001315 1.095030

18 H 2.849043 2.173473 4.049857 2.584278 1.090395

19 H 6.930204 5.740301 7.584176 7.456185 5.924946

20 H 7.129094 5.735103 7.879432 7.677531 5.582001

21 H 8.116396 6.851345 9.078884 8.262149 6.323558

22 H 7.978865 6.887724 8.856397 8.101631 6.664367

23 H 9.439299 8.231015 10.140868 9.852614 8.215663

24 H 9.573153 8.219976 10.356051 9.996586 7.956560

25 H 11.479651 10.236013 12.299937 11.736858 9.948352

26 H 10.674995 9.427941 11.610084 10.796224 8.921218

27 H 10.561226 9.443955 11.423339 10.670554 9.162020

6 7 8 9 10

6 S 0.000000

7 C 1.758351 0.000000

8 S 2.958541 1.791113 0.000000

9 S 3.055388 1.721821 3.093258 0.000000

10 C 4.342878 2.837849 1.838886 3.411581 0.000000

11 C 5.543471 4.206779 2.766074 4.911043 1.524911

12 C 6.805709 5.367568 4.168065 5.742347 2.533534

13 C 8.042508 6.706013 5.308130 7.210752 3.900070

14 H 2.423697 3.012711 4.458848 3.161529 5.781471

15 H 4.114170 5.678100 6.442494 6.700571 8.168285

16 H 3.015044 2.764401 3.202576 3.336376 4.724403

17 H 3.819799 4.219643 4.832115 4.716550 6.451036

18 H 3.048859 3.589916 3.751152 4.691599 5.550838

19 H 4.262059 2.906337 2.406129 3.425600 1.092491

20 H 4.750675 3.049885 2.417887 3.069855 1.090303

21 H 5.865746 4.530633 2.919380 5.234278 2.158954

22 H 5.508807 4.454687 2.943322 5.451899 2.157839

23 H 6.784565 5.417373 4.466084 5.741794 2.743199

24 H 7.096279 5.503830 4.463055 5.570338 2.766608

25 H 8.932414 7.541500 6.257584 7.887640 4.708429

26 H 8.315534 6.963640 5.437513 7.486507 4.234456

27 H 8.055238 6.899583 5.446837 7.617636 4.222571

11 12 13 14 15

11 C 0.000000

12 C 1.531421 0.000000

13 C 2.545567 1.527547 0.000000

14 H 7.109470 8.307023 9.631294 0.000000

15 H 9.117413 10.550321 11.590710 3.956304 0.000000

16 H 5.742490 7.065738 8.204298 2.477783 4.795994

17 H 7.446010 8.808121 9.910200 2.521998 3.830029

18 H 6.360073 7.828312 8.811292 3.078758 3.531307

19 H 2.171761 2.813015 4.221507 5.891087 8.262910

20 H 2.170259 2.779884 4.214398 5.764314 8.578427

21 H 1.096678 2.157367 2.781716 7.225566 9.164372

22 H 1.096066 2.158900 2.760339 7.350931 8.915107

23 H 2.157548 1.096498 2.158240 8.402590 10.670063

24 H 2.158100 1.096382 2.158682 8.317652 10.890524

25 H 3.500312 2.180563 1.094275 10.479965 12.587783

26 H 2.811344 2.179153 1.095017 9.770481 11.674414

27 H 2.816995 2.178610 1.094940 9.848375 11.476104

16 17 18 19 20

16 H 0.000000

17 H 1.766870 0.000000

18 H 1.770729 1.772707 0.000000

19 H 5.273793 6.932677 6.034042 0.000000

20 H 4.688524 6.446672 5.819241 1.767594 0.000000

21 H 5.525539 7.199210 6.138350 3.072995 2.529126

22 H 6.060599 7.672301 6.386835 2.503582 3.070892

23 H 7.462814 9.192021 8.212882 2.575016 3.070243

24 H 7.051827 8.816250 8.030243 3.157884 2.564079

25 H 9.130686 10.860782 9.824684 4.912177 4.890076

26 H 8.107090 9.778964 8.701774 4.788439 4.458690

27 H 8.476133 10.128682 8.880515 4.424927 4.771245

21 22 23 24 25

21 H 0.000000

22 H 1.757443 0.000000

23 H 3.060736 2.518450 0.000000

24 H 2.497542 3.062006 1.754150 0.000000

25 H 3.782952 3.771702 2.505342 2.500197 0.000000

26 H 2.600648 3.111572 3.077813 2.528098 1.765553

27 H 3.156772 2.584183 2.521120 3.077512 1.765860

26 27

26 H 0.000000

27 H 1.766348 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.89D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.126266 -0.403474 -0.175641

2 6 0 -2.845747 0.098595 0.428390

3 8 0 -4.916489 0.279588 -0.787281

4 8 0 -4.307091 -1.731714 -0.004881

5 6 0 -2.396843 -0.609859 1.693107

6 16 0 -1.545188 -0.031137 -0.954456

7 6 0 -0.111016 0.657870 -0.205981

8 16 0 1.116683 -0.576066 0.216210

9 16 0 -0.029144 2.295258 0.320257

10 6 0 2.702108 0.296689 -0.109713

11 6 0 3.874266 -0.669907 0.021025

12 6 0 5.219206 0.025795 -0.207860

13 6 0 6.402131 -0.936331 -0.116191

14 1 0 -2.969486 1.167172 0.597876

15 1 0 -5.137387 -1.972163 -0.449561

16 1 0 -1.471130 -0.161634 2.056852

17 1 0 -3.152611 -0.503407 2.478329

18 1 0 -2.223894 -1.672975 1.523298

19 1 0 2.648004 0.714250 -1.117806

20 1 0 2.794657 1.122940 0.595627

21 1 0 3.869218 -1.127307 1.017751

22 1 0 3.761117 -1.488764 -0.698719

23 1 0 5.213699 0.508454 -1.192399

24 1 0 5.341029 0.829981 0.527325

25 1 0 7.352942 -0.418582 -0.275347

26 1 0 6.449287 -1.416770 0.866671

27 1 0 6.328530 -1.729336 -0.867603

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3357161 0.1910760 0.1792158

Leave Link 202 at Sat Aug 17 17:34:07 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1100.2717986919 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0547477914 Hartrees.

Nuclear repulsion after empirical dispersion term = 1100.2170509004 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

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Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2321

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.72D-10

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 93

GePol: Fraction of low-weight points (<1% of avg) = 4.01%

GePol: Cavity surface area = 309.372 Ang\*\*2

GePol: Cavity volume = 320.053 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057044340 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1100.2113464665 Hartrees.

Leave Link 301 at Sat Aug 17 17:34:07 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.86D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:34:07 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:34:08 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999991 -0.004266 0.000256 -0.000279 Ang= -0.49 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7553 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.62929100108

Leave Link 401 at Sat Aug 17 17:34:08 2019, MaxMem= 1342177280 cpu: 7.5

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16161123.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.11D-15 for 2299.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.70D-15 for 877 759.

Iteration 1 A^-1\*A deviation from unit magnitude is 4.88D-15 for 2299.

Iteration 1 A^-1\*A deviation from orthogonality is 2.70D-10 for 1049 987.

Iteration 2 A\*A^-1 deviation from unit magnitude is 3.55D-15 for 1639.

Iteration 2 A\*A^-1 deviation from orthogonality is 3.48D-15 for 880 422.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.22D-15 for 391.

Iteration 2 A^-1\*A deviation from orthogonality is 1.40D-15 for 2289 73.

E= -1658.67542311970

DIIS: error= 1.05D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67542311970 IErMin= 1 ErrMin= 1.05D-03

ErrMax= 1.05D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.11D-03 BMatP= 3.11D-03

IDIUse=3 WtCom= 9.89D-01 WtEn= 1.05D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.428 Goal= None Shift= 0.000

Gap= 0.483 Goal= None Shift= 0.000

GapD= 0.428 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=1.51D-04 MaxDP=7.01D-03 OVMax= 9.08D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.51D-04 CP: 1.00D+00

E= -1658.67683650669 Delta-E= -0.001413386995 Rises=F Damp=F

DIIS: error= 1.89D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67683650669 IErMin= 2 ErrMin= 1.89D-04

ErrMax= 1.89D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.20D-05 BMatP= 3.11D-03

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.89D-03

Coeff-Com: -0.547D-01 0.105D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.546D-01 0.105D+01

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.04D-05 MaxDP=1.27D-03 DE=-1.41D-03 OVMax= 2.69D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.00D-05 CP: 1.00D+00 1.03D+00

E= -1658.67684638571 Delta-E= -0.000009879017 Rises=F Damp=F

DIIS: error= 2.19D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67684638571 IErMin= 2 ErrMin= 1.89D-04

ErrMax= 2.19D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.46D-05 BMatP= 6.20D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.19D-03

Coeff-Com: -0.375D-01 0.537D+00 0.501D+00

Coeff-En: 0.000D+00 0.228D+00 0.772D+00

Coeff: -0.375D-01 0.536D+00 0.501D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.70D-05 MaxDP=6.62D-04 DE=-9.88D-06 OVMax= 1.64D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.13D-05 CP: 1.00D+00 1.07D+00 6.14D-01

E= -1658.67685637984 Delta-E= -0.000009994132 Rises=F Damp=F

DIIS: error= 1.21D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67685637984 IErMin= 4 ErrMin= 1.21D-04

ErrMax= 1.21D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.31D-05 BMatP= 5.46D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.21D-03

Coeff-Com: -0.149D-01 0.193D+00 0.335D+00 0.487D+00

Coeff-En: 0.000D+00 0.000D+00 0.197D+00 0.803D+00

Coeff: -0.149D-01 0.193D+00 0.335D+00 0.487D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.38D-06 MaxDP=2.73D-04 DE=-9.99D-06 OVMax= 6.04D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.10D-06 CP: 1.00D+00 1.08D+00 6.76D-01 6.27D-01

E= -1658.67685935550 Delta-E= -0.000002975660 Rises=F Damp=F

DIIS: error= 1.19D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67685935550 IErMin= 5 ErrMin= 1.19D-05

ErrMax= 1.19D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.49D-07 BMatP= 1.31D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.242D-02 0.239D-01 0.878D-01 0.192D+00 0.699D+00

Coeff: -0.242D-02 0.239D-01 0.878D-01 0.192D+00 0.699D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.69D-06 MaxDP=7.31D-05 DE=-2.98D-06 OVMax= 2.44D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.14D-06 CP: 1.00D+00 1.08D+00 7.07D-01 6.99D-01 9.89D-01

E= -1658.67685944417 Delta-E= -0.000000088667 Rises=F Damp=F

DIIS: error= 1.06D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67685944417 IErMin= 6 ErrMin= 1.06D-05

ErrMax= 1.06D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.29D-07 BMatP= 3.49D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.111D-02-0.200D-01-0.406D-02 0.335D-01 0.422D+00 0.567D+00

Coeff: 0.111D-02-0.200D-01-0.406D-02 0.335D-01 0.422D+00 0.567D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=8.34D-07 MaxDP=3.99D-05 DE=-8.87D-08 OVMax= 8.61D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.66D-07 CP: 1.00D+00 1.08D+00 7.22D-01 7.26D-01 1.06D+00

CP: 9.16D-01

E= -1658.67685947612 Delta-E= -0.000000031953 Rises=F Damp=F

DIIS: error= 2.20D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67685947612 IErMin= 7 ErrMin= 2.20D-06

ErrMax= 2.20D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.04D-08 BMatP= 1.29D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.856D-03-0.125D-01-0.172D-01-0.194D-01 0.656D-01 0.233D+00

Coeff-Com: 0.750D+00

Coeff: 0.856D-03-0.125D-01-0.172D-01-0.194D-01 0.656D-01 0.233D+00

Coeff: 0.750D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.19D-07 MaxDP=1.51D-05 DE=-3.20D-08 OVMax= 4.83D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.45D-07 CP: 1.00D+00 1.08D+00 7.27D-01 7.31D-01 1.11D+00

CP: 1.08D+00 1.13D+00

E= -1658.67685947989 Delta-E= -0.000000003771 Rises=F Damp=F

DIIS: error= 1.94D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67685947989 IErMin= 8 ErrMin= 1.94D-06

ErrMax= 1.94D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.48D-09 BMatP= 1.04D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.302D-03-0.353D-02-0.988D-02-0.191D-01-0.383D-01 0.313D-01

Coeff-Com: 0.460D+00 0.579D+00

Coeff: 0.302D-03-0.353D-02-0.988D-02-0.191D-01-0.383D-01 0.313D-01

Coeff: 0.460D+00 0.579D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.83D-07 MaxDP=7.15D-06 DE=-3.77D-09 OVMax= 3.00D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 8.92D-08 CP: 1.00D+00 1.08D+00 7.28D-01 7.38D-01 1.12D+00

CP: 1.15D+00 1.29D+00 8.32D-01

E= -1658.67685948114 Delta-E= -0.000000001248 Rises=F Damp=F

DIIS: error= 9.52D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67685948114 IErMin= 9 ErrMin= 9.52D-07

ErrMax= 9.52D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.06D-10 BMatP= 4.48D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.140D-04 0.844D-03-0.222D-02-0.776D-02-0.371D-01-0.361D-01

Coeff-Com: 0.102D+00 0.354D+00 0.627D+00

Coeff: -0.140D-04 0.844D-03-0.222D-02-0.776D-02-0.371D-01-0.361D-01

Coeff: 0.102D+00 0.354D+00 0.627D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=9.84D-08 MaxDP=4.97D-06 DE=-1.25D-09 OVMax= 1.19D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 3.85D-08 CP: 1.00D+00 1.08D+00 7.30D-01 7.37D-01 1.13D+00

CP: 1.18D+00 1.37D+00 9.62D-01 7.91D-01

E= -1658.67685948136 Delta-E= -0.000000000222 Rises=F Damp=F

DIIS: error= 3.02D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67685948136 IErMin=10 ErrMin= 3.02D-07

ErrMax= 3.02D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.21D-10 BMatP= 9.06D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.462D-04 0.919D-03 0.569D-04-0.185D-02-0.139D-01-0.241D-01

Coeff-Com: -0.109D-01 0.114D+00 0.346D+00 0.590D+00

Coeff: -0.462D-04 0.919D-03 0.569D-04-0.185D-02-0.139D-01-0.241D-01

Coeff: -0.109D-01 0.114D+00 0.346D+00 0.590D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.53D-08 MaxDP=1.19D-06 DE=-2.22D-10 OVMax= 3.00D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.49D-08 CP: 1.00D+00 1.08D+00 7.30D-01 7.38D-01 1.13D+00

CP: 1.19D+00 1.39D+00 9.98D-01 8.74D-01 8.86D-01

E= -1658.67685948144 Delta-E= -0.000000000074 Rises=F Damp=F

DIIS: error= 5.15D-08 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67685948144 IErMin=11 ErrMin= 5.15D-08

ErrMax= 5.15D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.63D-12 BMatP= 1.21D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.118D-04 0.155D-03 0.276D-03 0.302D-03 0.108D-02-0.318D-02

Coeff-Com: -0.176D-01-0.983D-02 0.230D-01 0.186D+00 0.819D+00

Coeff: -0.118D-04 0.155D-03 0.276D-03 0.302D-03 0.108D-02-0.318D-02

Coeff: -0.176D-01-0.983D-02 0.230D-01 0.186D+00 0.819D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.13D-08 MaxDP=4.35D-07 DE=-7.41D-11 OVMax= 1.40D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 5.91D-09 CP: 1.00D+00 1.08D+00 7.30D-01 7.37D-01 1.13D+00

CP: 1.19D+00 1.40D+00 1.01D+00 9.14D-01 1.02D+00

CP: 1.09D+00

E= -1658.67685948142 Delta-E= 0.000000000019 Rises=F Damp=F

DIIS: error= 2.82D-08 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=11 EnMin= -1658.67685948144 IErMin=12 ErrMin= 2.82D-08

ErrMax= 2.82D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.51D-12 BMatP= 7.63D-12

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.296D-05-0.940D-04 0.106D-03 0.430D-03 0.291D-02 0.271D-02

Coeff-Com: -0.518D-02-0.225D-01-0.533D-01-0.265D-01 0.309D+00 0.792D+00

Coeff: 0.296D-05-0.940D-04 0.106D-03 0.430D-03 0.291D-02 0.271D-02

Coeff: -0.518D-02-0.225D-01-0.533D-01-0.265D-01 0.309D+00 0.792D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.32D-09 MaxDP=2.34D-07 DE= 1.86D-11 OVMax= 6.84D-07

Error on total polarization charges = 0.04183

SCF Done: E(UB3LYP) = -1658.67685948 A.U. after 12 cycles

NFock= 12 Conv=0.53D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655230542448D+03 PE=-6.143178476628D+03 EE= 1.729059728232D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.58

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:34:34 2019, MaxMem= 1342177280 cpu: 296.3

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 342

Leave Link 701 at Sat Aug 17 17:34:35 2019, MaxMem= 1342177280 cpu: 10.1

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:34:35 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:34:38 2019, MaxMem= 1342177280 cpu: 35.9

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.34044958D+00-2.91807686D+00 5.34323372D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000441029 -0.000136505 0.000165880

2 6 -0.000159665 -0.000041838 -0.000169976

3 8 -0.000246330 0.000000897 -0.000360579

4 8 -0.000082827 0.000114577 -0.000025626

5 6 0.000150326 0.000040477 -0.000071581

6 16 -0.000368965 0.000030876 0.000306778

7 6 -0.000052340 -0.000210300 0.000085863

8 16 -0.000316354 -0.000136519 0.000045484

9 16 -0.000023968 -0.000004156 0.000174535

10 6 0.000054438 0.000105803 -0.000003063

11 6 0.000022330 -0.000052910 -0.000070987

12 6 0.000028542 0.000102527 0.000120299

13 6 0.000055976 -0.000059846 -0.000109042

14 1 0.000191914 -0.000008461 -0.000016784

15 1 -0.000021998 0.000094268 0.000032841

16 1 0.000185334 0.000034639 -0.000018739

17 1 0.000032168 -0.000111443 0.000016216

18 1 0.000138676 0.000105603 -0.000090947

19 1 -0.000005714 0.000002803 0.000056246

20 1 0.000097700 0.000017883 0.000030548

21 1 0.000021805 0.000025736 -0.000046672

22 1 -0.000018058 0.000112828 -0.000036328

23 1 -0.000037571 -0.000027273 0.000031686

24 1 -0.000015348 -0.000074519 0.000028769

25 1 -0.000045930 0.000003580 0.000012898

26 1 0.000005623 0.000014993 -0.000054169

27 1 -0.000030795 0.000056279 -0.000033552

-------------------------------------------------------------------

Cartesian Forces: Max 0.000441029 RMS 0.000123222

Leave Link 716 at Sat Aug 17 17:34:38 2019, MaxMem= 1342177280 cpu: 0.3

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.001205545 RMS 0.000191978

Search for a local minimum.

Step number 12 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .19198D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 3 4 5 6

2 8 9 10 11

12

DE= -4.70D-05 DEPred=-1.55D-05 R= 3.03D+00

TightC=F SS= 1.41D+00 RLast= 8.57D-02 DXNew= 1.4142D-01 2.5711D-01

Trust test= 3.03D+00 RLast= 8.57D-02 DXMaxT set to 1.41D-01

ITU= 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Eigenvalues --- 0.00210 0.00270 0.00342 0.00381 0.00428

Eigenvalues --- 0.00491 0.00538 0.00936 0.01111 0.01961

Eigenvalues --- 0.02340 0.03080 0.03513 0.03614 0.04641

Eigenvalues --- 0.04831 0.04862 0.04971 0.05345 0.05451

Eigenvalues --- 0.05475 0.05627 0.05652 0.05838 0.08234

Eigenvalues --- 0.08338 0.08621 0.11281 0.12146 0.12205

Eigenvalues --- 0.13806 0.15863 0.15993 0.16000 0.16029

Eigenvalues --- 0.16049 0.16275 0.16663 0.17648 0.18938

Eigenvalues --- 0.20404 0.21909 0.21935 0.22150 0.23484

Eigenvalues --- 0.24769 0.24906 0.25367 0.25936 0.26619

Eigenvalues --- 0.27769 0.29125 0.29253 0.29471 0.29737

Eigenvalues --- 0.30202 0.32064 0.33544 0.33873 0.33878

Eigenvalues --- 0.33897 0.33950 0.34028 0.34040 0.34081

Eigenvalues --- 0.34110 0.34253 0.34431 0.34559 0.34610

Eigenvalues --- 0.35665 0.36201 0.52479 0.56813 1.03380

En-DIIS/RFO-DIIS IScMMF= 0 using points: 12 11 10 9 8

RFO step: Lambda=-1.41550757D-05.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 1.44D-06 SmlDif= 1.00D-05

RMS Error= 0.9340959799D-03 NUsed= 5 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.61128 0.20181 0.30564 1.17138 -1.29010

Iteration 1 RMS(Cart)= 0.01821083 RMS(Int)= 0.00008817

Iteration 2 RMS(Cart)= 0.00025403 RMS(Int)= 0.00002521

Iteration 3 RMS(Cart)= 0.00000002 RMS(Int)= 0.00002521

ITry= 1 IFail=0 DXMaxC= 7.08D-02 DCOld= 1.00D+10 DXMaxT= 1.41D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83878 -0.00001 0.00047 -0.00029 0.00018 2.83896

R2 2.28737 0.00031 0.00066 0.00066 0.00133 2.28870

R3 2.55363 -0.00016 0.00046 -0.00038 0.00008 2.55371

R4 2.86774 -0.00008 0.00026 -0.00014 0.00013 2.86786

R5 3.59572 -0.00082 -0.00011 -0.00056 -0.00067 3.59505

R6 2.05789 -0.00003 0.00009 0.00035 0.00044 2.05832

R7 1.83697 -0.00003 0.00022 0.00021 0.00043 1.83740

R8 2.06159 0.00017 0.00006 0.00039 0.00045 2.06203

R9 2.06931 0.00000 0.00014 0.00014 0.00028 2.06958

R10 2.06055 -0.00008 0.00007 0.00019 0.00026 2.06081

R11 3.32280 -0.00016 0.00071 -0.00089 -0.00018 3.32262

R12 3.38471 -0.00012 0.00039 -0.00081 -0.00042 3.38429

R13 3.25377 0.00005 0.00009 0.00042 0.00051 3.25428

R14 3.47499 0.00019 0.00025 0.00044 0.00069 3.47568

R15 2.88166 -0.00003 0.00032 -0.00020 0.00011 2.88178

R16 2.06451 -0.00004 0.00017 0.00014 0.00031 2.06482

R17 2.06037 0.00003 0.00024 0.00015 0.00039 2.06076

R18 2.89397 -0.00006 0.00018 0.00000 0.00018 2.89415

R19 2.07242 -0.00004 0.00012 0.00010 0.00022 2.07265

R20 2.07127 -0.00005 0.00012 0.00008 0.00020 2.07146

R21 2.88665 0.00000 0.00030 -0.00016 0.00015 2.88679

R22 2.07208 -0.00004 0.00010 0.00015 0.00025 2.07233

R23 2.07186 -0.00003 0.00013 0.00008 0.00021 2.07207

R24 2.06788 -0.00004 0.00015 0.00007 0.00021 2.06809

R25 2.06928 -0.00003 0.00016 0.00007 0.00023 2.06951

R26 2.06914 -0.00002 0.00016 0.00007 0.00023 2.06937

A1 2.17861 0.00028 0.00040 -0.00068 -0.00027 2.17834

A2 1.97334 0.00002 0.00012 0.00078 0.00091 1.97425

A3 2.13078 -0.00030 -0.00051 -0.00012 -0.00062 2.13015

A4 2.01665 0.00050 0.00015 0.00045 0.00060 2.01725

A5 1.84172 0.00007 0.00100 -0.00192 -0.00091 1.84081

A6 1.86887 -0.00002 0.00112 -0.00142 -0.00030 1.86856

A7 1.95159 -0.00057 -0.00135 0.00168 0.00034 1.95193

A8 1.94121 -0.00008 -0.00063 0.00123 0.00060 1.94181

A9 1.83141 0.00009 -0.00019 -0.00033 -0.00051 1.83091

A10 1.87509 -0.00012 0.00136 -0.00240 -0.00104 1.87405

A11 1.91460 -0.00013 -0.00093 0.00134 0.00041 1.91501

A12 1.92630 0.00016 0.00036 -0.00058 -0.00022 1.92609

A13 1.95228 -0.00009 0.00025 -0.00073 -0.00048 1.95180

A14 1.88243 0.00003 0.00018 0.00000 0.00018 1.88262

A15 1.89433 0.00000 -0.00020 0.00009 -0.00010 1.89422

A16 1.89223 0.00003 0.00034 -0.00010 0.00024 1.89246

A17 1.79407 -0.00121 -0.00062 0.00046 -0.00016 1.79390

A18 1.97083 -0.00033 -0.00087 0.00253 0.00181 1.97265

A19 2.14303 0.00016 -0.00005 0.00000 0.00011 2.14315

A20 2.15377 0.00013 -0.00018 -0.00015 -0.00017 2.15359

A21 1.79488 -0.00008 0.00043 -0.00191 -0.00148 1.79340

A22 1.92483 -0.00004 0.00011 0.00030 0.00041 1.92525

A23 1.87785 0.00003 0.00014 -0.00025 -0.00011 1.87774

A24 1.89462 0.00006 0.00031 -0.00021 0.00010 1.89472

A25 1.93848 -0.00008 -0.00003 -0.00022 -0.00025 1.93823

A26 1.93869 0.00003 -0.00039 0.00028 -0.00011 1.93857

A27 1.88757 0.00000 -0.00012 0.00009 -0.00004 1.88754

A28 1.95444 0.00005 0.00030 -0.00067 -0.00037 1.95407

A29 1.91639 0.00005 -0.00021 0.00043 0.00022 1.91661

A30 1.91549 -0.00009 0.00004 -0.00023 -0.00019 1.91529

A31 1.90641 -0.00006 -0.00029 0.00027 -0.00002 1.90639

A32 1.90912 0.00002 0.00000 -0.00002 -0.00002 1.90910

A33 1.85954 0.00003 0.00015 0.00027 0.00042 1.85996

A34 1.96600 0.00000 0.00006 0.00002 0.00008 1.96608

A35 1.90684 -0.00002 -0.00020 -0.00003 -0.00023 1.90661

A36 1.90771 -0.00002 -0.00001 -0.00016 -0.00017 1.90754

A37 1.91242 -0.00002 0.00003 -0.00027 -0.00024 1.91218

A38 1.91315 0.00003 -0.00005 0.00025 0.00020 1.91335

A39 1.85436 0.00003 0.00018 0.00020 0.00038 1.85473

A40 1.94564 -0.00002 0.00011 -0.00039 -0.00028 1.94536

A41 1.94288 0.00001 -0.00016 0.00003 -0.00012 1.94276

A42 1.94221 -0.00004 -0.00010 -0.00009 -0.00018 1.94202

A43 1.87625 0.00000 -0.00007 0.00029 0.00022 1.87646

A44 1.87682 0.00003 0.00010 0.00014 0.00024 1.87706

A45 1.87664 0.00002 0.00012 0.00004 0.00016 1.87681

D1 2.59161 0.00031 -0.00289 0.01120 0.00832 2.59992

D2 -1.52606 -0.00004 -0.00376 0.01220 0.00845 -1.51761

D3 0.41848 0.00008 -0.00305 0.01040 0.00735 0.42582

D4 -0.58182 0.00030 -0.00139 0.01015 0.00876 -0.57306

D5 1.58370 -0.00005 -0.00226 0.01115 0.00889 1.59258

D6 -2.75495 0.00007 -0.00155 0.00934 0.00779 -2.74716

D7 -3.10841 -0.00006 -0.00060 -0.00039 -0.00099 -3.10940

D8 0.00234 -0.00006 0.00086 -0.00143 -0.00056 0.00178

D9 -3.12626 -0.00013 0.00154 -0.00303 -0.00148 -3.12775

D10 -1.05444 -0.00007 0.00141 -0.00255 -0.00114 -1.05558

D11 1.05391 0.00001 0.00226 -0.00357 -0.00131 1.05259

D12 1.04995 -0.00015 0.00116 -0.00214 -0.00098 1.04897

D13 3.12178 -0.00009 0.00103 -0.00166 -0.00064 3.12114

D14 -1.05306 -0.00001 0.00187 -0.00268 -0.00081 -1.05387

D15 -0.99121 0.00016 0.00265 -0.00360 -0.00094 -0.99216

D16 1.08061 0.00022 0.00252 -0.00312 -0.00060 1.08001

D17 -3.09423 0.00030 0.00337 -0.00414 -0.00077 -3.09500

D18 3.08546 0.00031 -0.01040 0.00712 -0.00327 3.08219

D19 -0.99179 0.00063 -0.01037 0.00742 -0.00295 -0.99474

D20 1.11456 0.00027 -0.01197 0.00962 -0.00236 1.11220

D21 1.86207 0.00006 -0.01029 0.01720 0.00691 1.86898

D22 -1.09660 0.00027 -0.00699 0.00340 -0.00360 -1.10019

D23 2.51458 0.00017 0.02391 -0.04183 -0.01790 2.49668

D24 -0.81124 -0.00004 0.02066 -0.02791 -0.00728 -0.81852

D25 -3.01094 0.00021 -0.01426 0.02763 0.01337 -2.99757

D26 -0.89421 0.00011 -0.01414 0.02738 0.01324 -0.88097

D27 1.14461 0.00016 -0.01405 0.02724 0.01319 1.15781

D28 -3.11607 -0.00001 0.00094 0.00011 0.00105 -3.11502

D29 -0.99512 -0.00002 0.00063 0.00030 0.00093 -0.99419

D30 1.04335 0.00000 0.00071 0.00075 0.00146 1.04481

D31 1.08688 0.00003 0.00071 0.00038 0.00109 1.08797

D32 -3.07535 0.00002 0.00040 0.00057 0.00096 -3.07439

D33 -1.03688 0.00003 0.00048 0.00101 0.00149 -1.03539

D34 -1.01471 0.00006 0.00115 0.00023 0.00138 -1.01334

D35 1.10624 0.00005 0.00084 0.00042 0.00125 1.10749

D36 -3.13847 0.00006 0.00092 0.00086 0.00178 -3.13669

D37 -3.11563 0.00009 -0.00177 0.00492 0.00315 -3.11248

D38 -0.98597 0.00005 -0.00184 0.00457 0.00273 -0.98324

D39 1.03636 0.00006 -0.00174 0.00470 0.00296 1.03933

D40 1.04088 0.00005 -0.00150 0.00463 0.00313 1.04401

D41 -3.11265 0.00000 -0.00157 0.00428 0.00271 -3.10994

D42 -1.09032 0.00001 -0.00147 0.00441 0.00294 -1.08737

D43 -0.98822 0.00003 -0.00152 0.00416 0.00265 -0.98557

D44 1.14144 -0.00001 -0.00158 0.00381 0.00223 1.14367

D45 -3.11941 0.00000 -0.00149 0.00395 0.00246 -3.11695

D46 -3.13439 -0.00001 -0.00160 0.00295 0.00135 -3.13304

D47 -1.03948 -0.00002 -0.00172 0.00307 0.00135 -1.03812

D48 1.05362 -0.00001 -0.00174 0.00309 0.00135 1.05497

D49 1.02230 0.00003 -0.00140 0.00316 0.00176 1.02406

D50 3.11721 0.00002 -0.00152 0.00329 0.00177 3.11898

D51 -1.07288 0.00003 -0.00154 0.00330 0.00177 -1.07111

D52 -1.00627 -0.00001 -0.00160 0.00293 0.00133 -1.00494

D53 1.08865 -0.00001 -0.00172 0.00306 0.00134 1.08998

D54 -3.10145 -0.00001 -0.00174 0.00307 0.00133 -3.10011

Item Value Threshold Converged?

Maximum Force 0.001206 0.000450 NO

RMS Force 0.000192 0.000300 YES

Maximum Displacement 0.070805 0.001800 NO

RMS Displacement 0.018182 0.001200 NO

Predicted change in Energy=-2.810891D-06

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:34:38 2019, MaxMem= 1342177280 cpu: 0.6

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.107037 -0.384048 -0.230771

2 6 0 -2.838805 0.036285 0.456144

3 8 0 -4.883742 0.371816 -0.771354

4 8 0 -4.294253 -1.722375 -0.226509

5 6 0 -2.410560 -0.828259 1.627598

6 16 0 -1.514512 0.084952 -0.908804

7 6 0 -0.096641 0.677287 -0.054265

8 16 0 1.135837 -0.592335 0.222055

9 16 0 -0.029195 2.237580 0.671360

10 6 0 2.716730 0.322573 0.006273

11 6 0 3.893620 -0.647203 0.005379

12 6 0 5.234441 0.079496 -0.134825

13 6 0 6.422026 -0.880391 -0.178393

14 1 0 -2.968056 1.074768 0.758209

15 1 0 -5.116202 -1.902132 -0.713826

16 1 0 -1.491640 -0.431111 2.061802

17 1 0 -3.180180 -0.822499 2.406741

18 1 0 -2.233162 -1.861088 1.325848

19 1 0 2.656450 0.867499 -0.938881

20 1 0 2.809263 1.050670 0.812822

21 1 0 3.894707 -1.231357 0.933672

22 1 0 3.781249 -1.364962 -0.815467

23 1 0 5.221494 0.689150 -1.046283

24 1 0 5.356609 0.778854 0.700800

25 1 0 7.369774 -0.340893 -0.270045

26 1 0 6.475672 -1.488719 0.730667

27 1 0 6.348273 -1.565195 -1.029723

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.502313 0.000000

3 O 1.211128 2.408547 0.000000

4 O 1.351365 2.382693 2.242764 0.000000

5 C 2.555170 1.517608 3.648531 2.790243 0.000000

6 S 2.720456 1.902421 3.384212 3.385102 2.840809

7 C 4.152212 2.861969 4.850141 4.838181 3.232577

8 S 5.266514 4.030849 6.176713 5.564538 3.822061

9 S 4.931082 3.575742 5.397140 5.888814 3.998082

10 C 6.864350 5.581068 7.640307 7.306838 5.499292

11 C 8.008467 6.782028 8.870389 8.261418 6.512071

12 C 9.353464 8.094962 10.142398 9.697997 7.897860

13 C 10.540886 9.327696 11.390347 10.749413 9.015481

14 H 2.098452 1.089218 2.550207 3.248458 2.165214

15 H 1.885825 3.211358 2.286524 0.972312 3.735768

16 H 3.478277 2.147430 4.491973 3.841663 1.091181

17 H 2.829801 2.158443 3.798526 2.997489 1.095176

18 H 2.848880 2.173295 4.050888 2.584018 1.090532

19 H 6.914662 5.730170 7.558324 7.451657 5.927648

20 H 7.140218 5.749510 7.883703 7.696098 5.607208

21 H 8.130300 6.868416 9.085067 8.285299 6.356133

22 H 7.970516 6.885173 8.837444 8.104835 6.677958

23 H 9.425408 8.225081 10.113955 9.850732 8.228027

24 H 9.580228 8.232623 10.353632 10.012751 7.985655

25 H 11.476959 10.241323 12.284458 11.745633 9.974643

26 H 10.683557 9.442483 11.608356 10.814900 8.955770

27 H 10.552107 9.443249 11.400743 10.673951 9.182680

6 7 8 9 10

6 S 0.000000

7 C 1.758254 0.000000

8 S 2.960052 1.790892 0.000000

9 S 3.055633 1.722091 3.093153 0.000000

10 C 4.335578 2.836290 1.839250 3.413165 0.000000

11 C 5.533505 4.204761 2.766826 4.914671 1.524971

12 C 6.793190 5.365098 4.168605 5.745705 2.533350

13 C 8.028326 6.703341 5.309155 7.215405 3.900056

14 H 2.423109 3.010503 4.461909 3.161737 5.783424

15 H 4.118093 5.681938 6.455961 6.703253 8.174514

16 H 3.015186 2.766280 3.211588 3.345741 4.743797

17 H 3.819785 4.220677 4.842916 4.722746 6.468924

18 H 3.049131 3.593436 3.765402 4.699458 5.568760

19 H 4.243843 2.897971 2.406481 3.417995 1.092655

20 H 4.753065 3.055410 2.418434 3.079871 1.090508

21 H 5.864046 4.533188 2.919951 5.243981 2.159258

22 H 5.491452 4.448397 2.944760 5.450546 2.157830

23 H 6.764446 5.409880 4.465812 5.737393 2.741550

24 H 7.091165 5.506212 4.463661 5.579931 2.767584

25 H 8.917392 7.538607 6.258382 7.891736 4.708222

26 H 8.307066 6.964409 5.438385 7.496807 4.234993

27 H 8.034986 6.893270 5.448201 7.617538 4.221974

11 12 13 14 15

11 C 0.000000

12 C 1.531518 0.000000

13 C 2.545777 1.527625 0.000000

14 H 7.114390 8.310778 9.637090 0.000000

15 H 9.125185 10.554520 11.595746 3.955167 0.000000

16 H 5.768587 7.094085 8.236894 2.479281 4.796401

17 H 7.472343 8.836232 9.944276 2.522355 3.827757

18 H 6.383935 7.852676 8.839501 3.079210 3.531836

19 H 2.171760 2.813092 4.220547 5.878618 8.254430

20 H 2.170385 2.778975 4.214684 5.777627 8.594340

21 H 1.096797 2.157523 2.783380 7.241997 9.184806

22 H 1.096172 2.159049 2.759415 7.347235 8.914231

23 H 2.157564 1.096632 2.158232 8.394857 10.662703

24 H 2.158144 1.096493 2.158978 8.330120 10.902688

25 H 3.500475 2.180518 1.094388 10.484852 12.591028

26 H 2.810904 2.179227 1.095139 9.785511 11.688841

27 H 2.817706 2.178640 1.095062 9.846832 11.473775

16 17 18 19 20

16 H 0.000000

17 H 1.767296 0.000000

18 H 1.770966 1.773088 0.000000

19 H 5.281774 6.936536 6.040074 0.000000

20 H 4.717349 6.474779 5.845304 1.767871 0.000000

21 H 5.561097 7.238171 6.172613 3.073260 2.529909

22 H 6.078990 7.690149 6.403477 2.502855 3.071052

23 H 7.482068 9.208506 8.228160 2.573479 3.066893

24 H 7.086244 8.851629 8.060063 3.160264 2.564255

25 H 9.163531 10.894891 9.852626 4.911514 4.889510

26 H 8.146687 9.822858 8.737087 4.788069 4.460696

27 H 8.503406 10.156392 8.903781 4.422195 4.770988

21 22 23 24 25

21 H 0.000000

22 H 1.757899 0.000000

23 H 3.060871 2.519316 0.000000

24 H 2.496464 3.062151 1.754595 0.000000

25 H 3.783906 3.771433 2.505721 2.499841 0.000000

26 H 2.601697 3.108980 3.077925 2.528850 1.765884

27 H 3.160120 2.583721 2.520313 3.077772 1.766208

26 27

26 H 0.000000

27 H 1.766650 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 7.43D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.125125 -0.403274 -0.192051

2 6 0 -2.850379 0.102254 0.421469

3 8 0 -4.902743 0.273924 -0.827302

4 8 0 -4.317502 -1.727113 -0.000661

5 6 0 -2.417108 -0.593250 1.698844

6 16 0 -1.535724 -0.045563 -0.945659

7 6 0 -0.109474 0.652857 -0.191023

8 16 0 1.120012 -0.572027 0.250922

9 16 0 -0.030769 2.298473 0.310326

10 6 0 2.702859 0.296372 -0.100244

11 6 0 3.875937 -0.669814 0.025887

12 6 0 5.218530 0.023863 -0.222714

13 6 0 6.402035 -0.938508 -0.140284

14 1 0 -2.973426 1.173242 0.577163

15 1 0 -5.143615 -1.968836 -0.452874

16 1 0 -1.493563 -0.144093 2.067622

17 1 0 -3.181095 -0.475592 2.474661

18 1 0 -2.245891 -1.658829 1.542360

19 1 0 2.637923 0.705013 -1.111526

20 1 0 2.803998 1.128989 0.596698

21 1 0 3.881410 -1.119358 1.026309

22 1 0 3.754898 -1.494082 -0.686521

23 1 0 5.201419 0.501056 -1.209930

24 1 0 5.349401 0.831916 0.506822

25 1 0 7.351190 -0.421567 -0.312218

26 1 0 6.459834 -1.414918 0.844105

27 1 0 6.319523 -1.734564 -0.887712

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3324983 0.1909509 0.1792000

Leave Link 202 at Sat Aug 17 17:34:38 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1100.0136558595 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0547189860 Hartrees.

Nuclear repulsion after empirical dispersion term = 1099.9589368735 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2324

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.47D-10

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 95

GePol: Fraction of low-weight points (<1% of avg) = 4.09%

GePol: Cavity surface area = 309.410 Ang\*\*2

GePol: Cavity volume = 320.166 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057259016 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1099.9532109719 Hartrees.

Leave Link 301 at Sat Aug 17 17:34:38 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.86D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:34:38 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:34:38 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999995 0.003092 0.000358 0.000134 Ang= 0.36 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7553 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.62909946465

Leave Link 401 at Sat Aug 17 17:34:39 2019, MaxMem= 1342177280 cpu: 7.5

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16202928.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.55D-15 for 2312.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.72D-15 for 1756 193.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.44D-15 for 2318.

Iteration 1 A^-1\*A deviation from orthogonality is 5.28D-13 for 1037 1014.

E= -1658.67616139392

DIIS: error= 9.04D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67616139392 IErMin= 1 ErrMin= 9.04D-04

ErrMax= 9.04D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.52D-03 BMatP= 1.52D-03

IDIUse=3 WtCom= 9.91D-01 WtEn= 9.04D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.428 Goal= None Shift= 0.000

Gap= 0.483 Goal= None Shift= 0.000

RMSDP=9.20D-05 MaxDP=2.65D-03 OVMax= 5.78D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 9.20D-05 CP: 1.00D+00

E= -1658.67684317337 Delta-E= -0.000681779446 Rises=F Damp=F

DIIS: error= 1.43D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67684317337 IErMin= 2 ErrMin= 1.43D-04

ErrMax= 1.43D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.68D-05 BMatP= 1.52D-03

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.43D-03

Coeff-Com: -0.693D-01 0.107D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.692D-01 0.107D+01

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.45D-05 MaxDP=4.07D-04 DE=-6.82D-04 OVMax= 1.02D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.33D-05 CP: 1.00D+00 1.06D+00

E= -1658.67685083738 Delta-E= -0.000007664013 Rises=F Damp=F

DIIS: error= 5.95D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67685083738 IErMin= 3 ErrMin= 5.95D-05

ErrMax= 5.95D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.23D-06 BMatP= 2.68D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.294D-01 0.394D+00 0.636D+00

Coeff: -0.294D-01 0.394D+00 0.636D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=9.11D-06 MaxDP=3.81D-04 DE=-7.66D-06 OVMax= 1.02D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 7.23D-06 CP: 1.00D+00 1.09D+00 6.43D-01

E= -1658.67685172792 Delta-E= -0.000000890534 Rises=F Damp=F

DIIS: error= 4.72D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67685172792 IErMin= 4 ErrMin= 4.72D-05

ErrMax= 4.72D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.17D-06 BMatP= 8.23D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.121D-01 0.153D+00 0.440D+00 0.419D+00

Coeff: -0.121D-01 0.153D+00 0.440D+00 0.419D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.01D-06 MaxDP=1.83D-04 DE=-8.91D-07 OVMax= 4.22D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.22D-06 CP: 1.00D+00 1.09D+00 7.61D-01 5.94D-01

E= -1658.67685299749 Delta-E= -0.000001269577 Rises=F Damp=F

DIIS: error= 8.13D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67685299749 IErMin= 5 ErrMin= 8.13D-06

ErrMax= 8.13D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.17D-07 BMatP= 5.17D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.137D-02 0.109D-01 0.114D+00 0.167D+00 0.710D+00

Coeff: -0.137D-02 0.109D-01 0.114D+00 0.167D+00 0.710D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=9.56D-07 MaxDP=3.51D-05 DE=-1.27D-06 OVMax= 8.32D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 6.90D-07 CP: 1.00D+00 1.09D+00 7.95D-01 6.55D-01 9.22D-01

E= -1658.67685302522 Delta-E= -0.000000027728 Rises=F Damp=F

DIIS: error= 5.15D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67685302522 IErMin= 6 ErrMin= 5.15D-06

ErrMax= 5.15D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.78D-08 BMatP= 1.17D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.108D-02-0.188D-01 0.455D-03 0.331D-01 0.416D+00 0.568D+00

Coeff: 0.108D-02-0.188D-01 0.455D-03 0.331D-01 0.416D+00 0.568D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.52D-07 MaxDP=1.62D-05 DE=-2.77D-08 OVMax= 5.48D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 3.06D-07 CP: 1.00D+00 1.10D+00 8.03D-01 6.86D-01 1.00D+00

CP: 8.38D-01

E= -1658.67685303505 Delta-E= -0.000000009828 Rises=F Damp=F

DIIS: error= 2.02D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67685303505 IErMin= 7 ErrMin= 2.02D-06

ErrMax= 2.02D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.86D-09 BMatP= 3.78D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.627D-03-0.933D-02-0.134D-01-0.818D-02 0.884D-01 0.238D+00

Coeff-Com: 0.704D+00

Coeff: 0.627D-03-0.933D-02-0.134D-01-0.818D-02 0.884D-01 0.238D+00

Coeff: 0.704D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.96D-07 MaxDP=8.38D-06 DE=-9.83D-09 OVMax= 2.03D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.05D-07 CP: 1.00D+00 1.10D+00 8.07D-01 6.91D-01 1.05D+00

CP: 9.53D-01 1.13D+00

E= -1658.67685303591 Delta-E= -0.000000000860 Rises=F Damp=F

DIIS: error= 1.63D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67685303591 IErMin= 8 ErrMin= 1.63D-06

ErrMax= 1.63D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.39D-09 BMatP= 2.86D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.139D-03-0.140D-02-0.863D-02-0.135D-01-0.397D-01 0.223D-01

Coeff-Com: 0.462D+00 0.579D+00

Coeff: 0.139D-03-0.140D-02-0.863D-02-0.135D-01-0.397D-01 0.223D-01

Coeff: 0.462D+00 0.579D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.09D-07 MaxDP=5.14D-06 DE=-8.60D-10 OVMax= 1.32D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 5.07D-08 CP: 1.00D+00 1.10D+00 8.09D-01 6.98D-01 1.07D+00

CP: 1.03D+00 1.27D+00 7.73D-01

E= -1658.67685303626 Delta-E= -0.000000000353 Rises=F Damp=F

DIIS: error= 4.46D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67685303626 IErMin= 9 ErrMin= 4.46D-07

ErrMax= 4.46D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.01D-10 BMatP= 1.39D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.689D-04 0.152D-02-0.181D-02-0.604D-02-0.439D-01-0.417D-01

Coeff-Com: 0.923D-01 0.328D+00 0.672D+00

Coeff: -0.689D-04 0.152D-02-0.181D-02-0.604D-02-0.439D-01-0.417D-01

Coeff: 0.923D-01 0.328D+00 0.672D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.88D-08 MaxDP=2.14D-06 DE=-3.53D-10 OVMax= 5.54D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.82D-08 CP: 1.00D+00 1.10D+00 8.10D-01 7.00D-01 1.07D+00

CP: 1.06D+00 1.36D+00 9.11D-01 8.69D-01

E= -1658.67685303635 Delta-E= -0.000000000084 Rises=F Damp=F

DIIS: error= 1.36D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67685303635 IErMin=10 ErrMin= 1.36D-07

ErrMax= 1.36D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.93D-11 BMatP= 2.01D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.553D-04 0.103D-02-0.570D-04-0.188D-02-0.196D-01-0.259D-01

Coeff-Com: -0.458D-02 0.118D+00 0.365D+00 0.568D+00

Coeff: -0.553D-04 0.103D-02-0.570D-04-0.188D-02-0.196D-01-0.259D-01

Coeff: -0.458D-02 0.118D+00 0.365D+00 0.568D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.35D-08 MaxDP=6.20D-07 DE=-8.37D-11 OVMax= 1.61D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 6.98D-09 CP: 1.00D+00 1.10D+00 8.10D-01 7.01D-01 1.07D+00

CP: 1.07D+00 1.38D+00 9.40D-01 9.74D-01 8.35D-01

E= -1658.67685303634 Delta-E= 0.000000000010 Rises=F Damp=F

DIIS: error= 4.98D-08 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=10 EnMin= -1658.67685303635 IErMin=11 ErrMin= 4.98D-08

ErrMax= 4.98D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.77D-12 BMatP= 2.93D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.862D-05 0.116D-03 0.253D-03 0.278D-03 0.250D-03-0.228D-02

Coeff-Com: -0.179D-01-0.104D-01 0.161D-01 0.233D+00 0.781D+00

Coeff: -0.862D-05 0.116D-03 0.253D-03 0.278D-03 0.250D-03-0.228D-02

Coeff: -0.179D-01-0.104D-01 0.161D-01 0.233D+00 0.781D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.85D-09 MaxDP=2.86D-07 DE= 1.00D-11 OVMax= 6.67D-07

Error on total polarization charges = 0.04185

SCF Done: E(UB3LYP) = -1658.67685304 A.U. after 11 cycles

NFock= 11 Conv=0.58D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7553 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655223418291D+03 PE=-6.142655559921D+03 EE= 1.728802077621D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.59

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7553, after 0.7500

Leave Link 502 at Sat Aug 17 17:35:02 2019, MaxMem= 1342177280 cpu: 267.1

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 343

Leave Link 701 at Sat Aug 17 17:35:03 2019, MaxMem= 1342177280 cpu: 10.2

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:35:03 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:35:06 2019, MaxMem= 1342177280 cpu: 36.0

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.32511763D+00-2.90901739D+00 5.33581182D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000247925 0.000360782 -0.000187536

2 6 -0.000213477 0.000100261 -0.000225529

3 8 0.000463812 -0.000600099 0.000175897

4 8 -0.000203092 0.000290032 -0.000131517

5 6 0.000079058 0.000050213 -0.000087956

6 16 -0.000316099 -0.000063297 0.000295533

7 6 -0.000014869 -0.000075722 0.000086451

8 16 -0.000402424 -0.000008064 0.000015746

9 16 -0.000030726 -0.000180534 0.000086358

10 6 0.000151790 0.000120396 0.000057523

11 6 0.000032763 -0.000045657 -0.000090768

12 6 0.000033553 0.000109572 0.000120665

13 6 0.000024587 -0.000033895 -0.000105090

14 1 0.000221789 -0.000148124 0.000008464

15 1 0.000146307 0.000074531 0.000111425

16 1 0.000063881 0.000020272 -0.000085052

17 1 0.000117599 -0.000133960 -0.000043442

18 1 0.000133513 0.000169227 -0.000028038

19 1 -0.000043592 -0.000080128 0.000168627

20 1 0.000111132 -0.000038693 -0.000075999

21 1 0.000033726 0.000036561 -0.000119565

22 1 -0.000021753 0.000158054 0.000039661

23 1 -0.000035104 -0.000053743 0.000109695

24 1 -0.000013334 -0.000111970 -0.000046192

25 1 -0.000094118 -0.000063872 0.000020675

26 1 0.000028270 0.000057279 -0.000111162

27 1 -0.000005266 0.000090577 0.000041124

-------------------------------------------------------------------

Cartesian Forces: Max 0.000600099 RMS 0.000156088

Leave Link 716 at Sat Aug 17 17:35:06 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.001326970 RMS 0.000206217

Search for a local minimum.

Step number 13 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .20622D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 3 4 5 6

2 8 9 10 11

12 13

DE= 6.45D-06 DEPred=-2.81D-06 R=-2.29D+00

Trust test=-2.29D+00 RLast= 3.91D-02 DXMaxT set to 7.07D-02

ITU= -1 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Eigenvalues --- 0.00084 0.00290 0.00342 0.00380 0.00439

Eigenvalues --- 0.00491 0.00727 0.01090 0.01226 0.01692

Eigenvalues --- 0.02340 0.02646 0.03511 0.03612 0.04651

Eigenvalues --- 0.04836 0.04841 0.04984 0.05318 0.05454

Eigenvalues --- 0.05477 0.05627 0.05700 0.05814 0.08229

Eigenvalues --- 0.08332 0.08651 0.11291 0.12140 0.12221

Eigenvalues --- 0.13801 0.15714 0.15991 0.16000 0.16025

Eigenvalues --- 0.16073 0.16256 0.16425 0.17684 0.18921

Eigenvalues --- 0.20363 0.21889 0.21944 0.22635 0.23439

Eigenvalues --- 0.24044 0.24850 0.25260 0.25780 0.26462

Eigenvalues --- 0.27781 0.29117 0.29449 0.29698 0.30035

Eigenvalues --- 0.30350 0.31858 0.33579 0.33871 0.33878

Eigenvalues --- 0.33895 0.33957 0.34028 0.34040 0.34091

Eigenvalues --- 0.34136 0.34258 0.34457 0.34552 0.34612

Eigenvalues --- 0.36425 0.38957 0.52530 0.57531 1.09447

En-DIIS/RFO-DIIS IScMMF= 0 using points: 13 12 11 10 9

RFO step: Lambda=-1.31685569D-05.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= -2.93D-04 SmlDif= 1.00D-05

RMS Error= 0.7800139840D-03 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 2.13071 -1.33551 0.03536 0.12101 0.04843

Iteration 1 RMS(Cart)= 0.04704519 RMS(Int)= 0.00067559

Iteration 2 RMS(Cart)= 0.00105364 RMS(Int)= 0.00000853

Iteration 3 RMS(Cart)= 0.00000043 RMS(Int)= 0.00000853

ITry= 1 IFail=0 DXMaxC= 1.65D-01 DCOld= 1.00D+10 DXMaxT= 7.07D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83896 -0.00015 -0.00012 0.00145 0.00133 2.84029

R2 2.28870 -0.00076 0.00048 -0.00093 -0.00046 2.28824

R3 2.55371 -0.00032 -0.00035 0.00037 0.00002 2.55373

R4 2.86786 -0.00018 -0.00009 -0.00078 -0.00087 2.86700

R5 3.59505 -0.00074 -0.00164 -0.00089 -0.00253 3.59252

R6 2.05832 -0.00017 0.00013 0.00006 0.00019 2.05851

R7 1.83740 -0.00020 0.00011 0.00001 0.00012 1.83752

R8 2.06203 0.00004 0.00030 0.00007 0.00038 2.06241

R9 2.06958 -0.00011 0.00007 -0.00002 0.00005 2.06963

R10 2.06081 -0.00016 -0.00003 0.00002 -0.00001 2.06079

R11 3.32262 -0.00016 -0.00025 -0.00051 -0.00076 3.32186

R12 3.38429 -0.00018 -0.00045 -0.00145 -0.00191 3.38239

R13 3.25428 -0.00014 0.00022 0.00055 0.00076 3.25504

R14 3.47568 0.00022 0.00068 0.00199 0.00267 3.47834

R15 2.88178 -0.00008 -0.00013 -0.00009 -0.00021 2.88157

R16 2.06482 -0.00018 0.00001 -0.00020 -0.00019 2.06463

R17 2.06076 -0.00008 0.00013 0.00004 0.00017 2.06093

R18 2.89415 -0.00008 -0.00004 0.00013 0.00009 2.89424

R19 2.07265 -0.00011 -0.00001 0.00007 0.00006 2.07271

R20 2.07146 -0.00014 -0.00005 -0.00006 -0.00011 2.07136

R21 2.88679 -0.00005 -0.00005 -0.00021 -0.00026 2.88653

R22 2.07233 -0.00012 0.00001 0.00007 0.00009 2.07242

R23 2.07207 -0.00011 -0.00002 -0.00001 -0.00003 2.07205

R24 2.06809 -0.00012 -0.00003 0.00009 0.00006 2.06816

R25 2.06951 -0.00010 0.00000 0.00008 0.00008 2.06959

R26 2.06937 -0.00010 0.00000 0.00003 0.00003 2.06940

A1 2.17834 0.00020 0.00016 -0.00143 -0.00127 2.17707

A2 1.97425 0.00000 0.00053 0.00102 0.00156 1.97581

A3 2.13015 -0.00020 -0.00071 0.00052 -0.00020 2.12996

A4 2.01725 0.00043 0.00088 0.00210 0.00298 2.02023

A5 1.84081 0.00017 -0.00048 -0.00192 -0.00241 1.83840

A6 1.86856 -0.00002 0.00038 -0.00098 -0.00061 1.86796

A7 1.95193 -0.00062 -0.00045 -0.00014 -0.00059 1.95134

A8 1.94181 -0.00008 0.00065 -0.00081 -0.00015 1.94165

A9 1.83091 0.00011 -0.00120 0.00167 0.00047 1.83138

A10 1.87405 -0.00002 -0.00123 0.00083 -0.00040 1.87364

A11 1.91501 -0.00019 0.00043 -0.00062 -0.00020 1.91481

A12 1.92609 0.00021 0.00027 0.00059 0.00085 1.92694

A13 1.95180 -0.00003 -0.00065 0.00112 0.00046 1.95226

A14 1.88262 0.00003 0.00007 -0.00011 -0.00004 1.88257

A15 1.89422 0.00001 -0.00036 -0.00047 -0.00083 1.89339

A16 1.89246 -0.00002 0.00027 -0.00056 -0.00029 1.89217

A17 1.79390 -0.00133 -0.00102 -0.00048 -0.00150 1.79240

A18 1.97265 -0.00018 0.00134 0.00338 0.00477 1.97742

A19 2.14315 0.00009 -0.00003 -0.00125 -0.00122 2.14192

A20 2.15359 0.00005 -0.00041 -0.00240 -0.00276 2.15083

A21 1.79340 -0.00006 -0.00136 -0.00179 -0.00315 1.79025

A22 1.92525 0.00015 0.00036 0.00284 0.00320 1.92844

A23 1.87774 -0.00007 -0.00017 -0.00203 -0.00220 1.87554

A24 1.89472 0.00002 0.00032 0.00037 0.00068 1.89540

A25 1.93823 -0.00009 -0.00024 -0.00065 -0.00089 1.93733

A26 1.93857 -0.00002 -0.00016 -0.00018 -0.00034 1.93823

A27 1.88754 0.00001 -0.00010 -0.00045 -0.00055 1.88699

A28 1.95407 -0.00001 -0.00027 -0.00111 -0.00139 1.95268

A29 1.91661 0.00008 0.00021 0.00091 0.00112 1.91773

A30 1.91529 -0.00008 -0.00026 -0.00015 -0.00040 1.91489

A31 1.90639 -0.00005 -0.00003 -0.00039 -0.00042 1.90597

A32 1.90910 0.00006 0.00003 0.00074 0.00077 1.90987

A33 1.85996 0.00001 0.00036 0.00006 0.00042 1.86037

A34 1.96608 0.00003 0.00004 0.00075 0.00079 1.96687

A35 1.90661 -0.00003 -0.00030 -0.00012 -0.00042 1.90619

A36 1.90754 -0.00001 -0.00005 -0.00033 -0.00038 1.90716

A37 1.91218 -0.00002 -0.00025 -0.00012 -0.00036 1.91182

A38 1.91335 0.00001 0.00024 0.00013 0.00037 1.91371

A39 1.85473 0.00002 0.00034 -0.00038 -0.00004 1.85469

A40 1.94536 0.00002 -0.00022 0.00018 -0.00004 1.94532

A41 1.94276 0.00002 -0.00005 0.00028 0.00023 1.94299

A42 1.94202 -0.00002 -0.00009 0.00028 0.00018 1.94221

A43 1.87646 -0.00003 0.00007 -0.00049 -0.00042 1.87604

A44 1.87706 0.00000 0.00019 -0.00033 -0.00014 1.87692

A45 1.87681 0.00001 0.00012 0.00004 0.00016 1.87696

D1 2.59992 0.00027 0.00769 0.01384 0.02153 2.62145

D2 -1.51761 -0.00010 0.00732 0.01357 0.02089 -1.49673

D3 0.42582 0.00009 0.00591 0.01420 0.02012 0.44594

D4 -0.57306 0.00026 0.00713 0.01768 0.02480 -0.54826

D5 1.59258 -0.00012 0.00676 0.01740 0.02416 1.61674

D6 -2.74716 0.00007 0.00535 0.01804 0.02339 -2.72377

D7 -3.10940 -0.00003 -0.00096 -0.00016 -0.00112 -3.11052

D8 0.00178 -0.00004 -0.00148 0.00352 0.00203 0.00381

D9 -3.12775 -0.00009 -0.00086 -0.00237 -0.00323 -3.13098

D10 -1.05558 -0.00004 -0.00035 -0.00253 -0.00288 -1.05846

D11 1.05259 0.00006 -0.00027 -0.00209 -0.00236 1.05024

D12 1.04897 -0.00015 -0.00052 -0.00126 -0.00178 1.04720

D13 3.12114 -0.00011 -0.00001 -0.00142 -0.00143 3.11972

D14 -1.05387 -0.00001 0.00007 -0.00097 -0.00090 -1.05477

D15 -0.99216 0.00015 0.00085 -0.00274 -0.00189 -0.99405

D16 1.08001 0.00020 0.00136 -0.00290 -0.00154 1.07846

D17 -3.09500 0.00030 0.00144 -0.00246 -0.00102 -3.09602

D18 3.08219 0.00025 0.01121 -0.00265 0.00856 3.09075

D19 -0.99474 0.00052 0.01169 -0.00146 0.01022 -0.98452

D20 1.11220 0.00015 0.01148 -0.00147 0.01001 1.12221

D21 1.86898 -0.00002 0.00556 0.00083 0.00638 1.87536

D22 -1.10019 0.00028 -0.00105 0.00268 0.00163 -1.09857

D23 2.49668 0.00028 -0.01160 -0.00090 -0.01249 2.48420

D24 -0.81852 -0.00001 -0.00489 -0.00262 -0.00752 -0.82604

D25 -2.99757 0.00020 0.01191 0.04577 0.05768 -2.93989

D26 -0.88097 0.00014 0.01172 0.04540 0.05711 -0.82385

D27 1.15781 0.00013 0.01168 0.04397 0.05565 1.21346

D28 -3.11502 -0.00002 0.00075 0.00917 0.00992 -3.10510

D29 -0.99419 -0.00004 0.00067 0.00856 0.00923 -0.98496

D30 1.04481 -0.00002 0.00107 0.00908 0.01015 1.05497

D31 1.08797 0.00004 0.00089 0.01028 0.01116 1.09913

D32 -3.07439 0.00002 0.00081 0.00967 0.01048 -3.06391

D33 -1.03539 0.00003 0.00121 0.01019 0.01140 -1.02399

D34 -1.01334 0.00009 0.00128 0.01140 0.01268 -1.00066

D35 1.10749 0.00007 0.00120 0.01079 0.01199 1.11948

D36 -3.13669 0.00009 0.00160 0.01131 0.01292 -3.12377

D37 -3.11248 0.00009 0.00275 0.00692 0.00968 -3.10280

D38 -0.98324 0.00006 0.00226 0.00719 0.00944 -0.97380

D39 1.03933 0.00006 0.00246 0.00648 0.00895 1.04827

D40 1.04401 0.00003 0.00269 0.00677 0.00947 1.05348

D41 -3.10994 0.00001 0.00219 0.00704 0.00923 -3.10071

D42 -1.08737 0.00000 0.00240 0.00634 0.00874 -1.07864

D43 -0.98557 0.00001 0.00227 0.00651 0.00877 -0.97679

D44 1.14367 -0.00001 0.00177 0.00677 0.00854 1.15221

D45 -3.11695 -0.00001 0.00197 0.00607 0.00804 -3.10891

D46 -3.13304 -0.00001 0.00041 0.00459 0.00500 -3.12804

D47 -1.03812 -0.00003 0.00032 0.00428 0.00460 -1.03352

D48 1.05497 -0.00002 0.00038 0.00470 0.00508 1.06005

D49 1.02406 0.00002 0.00094 0.00432 0.00526 1.02933

D50 3.11898 0.00001 0.00085 0.00401 0.00486 3.12384

D51 -1.07111 0.00002 0.00091 0.00443 0.00534 -1.06577

D52 -1.00494 0.00000 0.00054 0.00477 0.00531 -0.99962

D53 1.08998 -0.00001 0.00045 0.00446 0.00491 1.09489

D54 -3.10011 0.00000 0.00051 0.00488 0.00539 -3.09472

Item Value Threshold Converged?

Maximum Force 0.001327 0.000450 NO

RMS Force 0.000206 0.000300 YES

Maximum Displacement 0.164904 0.001800 NO

RMS Displacement 0.047054 0.001200 NO

Predicted change in Energy=-2.284659D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:35:06 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.094717 -0.403226 -0.264937

2 6 0 -2.841046 0.038889 0.436424

3 8 0 -4.849804 0.334088 -0.858618

4 8 0 -4.296599 -1.738037 -0.203773

5 6 0 -2.431274 -0.790187 1.639112

6 16 0 -1.493182 0.052496 -0.904168

7 6 0 -0.089980 0.657330 -0.035117

8 16 0 1.140480 -0.602098 0.286582

9 16 0 -0.032862 2.232315 0.659969

10 6 0 2.720619 0.314328 0.059965

11 6 0 3.897424 -0.654233 0.012923

12 6 0 5.235089 0.079066 -0.123533

13 6 0 6.422765 -0.875896 -0.226902

14 1 0 -2.978756 1.085151 0.706582

15 1 0 -5.107518 -1.931917 -0.704107

16 1 0 -1.520196 -0.378524 2.076811

17 1 0 -3.213496 -0.764226 2.405221

18 1 0 -2.246299 -1.830881 1.370810

19 1 0 2.641121 0.879437 -0.871706

20 1 0 2.830955 1.025362 0.879514

21 1 0 3.912917 -1.266737 0.922667

22 1 0 3.773483 -1.346116 -0.828149

23 1 0 5.204531 0.723723 -1.010205

24 1 0 5.371738 0.745655 0.736265

25 1 0 7.368410 -0.331247 -0.309787

26 1 0 6.491610 -1.522701 0.654189

27 1 0 6.336748 -1.523449 -1.105808

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.503018 0.000000

3 O 1.210886 2.408191 0.000000

4 O 1.351377 2.384524 2.242445 0.000000

5 C 2.557770 1.517149 3.654030 2.788204 0.000000

6 S 2.717403 1.901081 3.368721 3.399369 2.838733

7 C 4.149157 2.858878 4.841338 4.843745 3.221801

8 S 5.267923 4.035575 6.170205 5.576077 3.823891

9 S 4.929522 3.570292 5.395581 5.889754 3.980781

10 C 6.860703 5.581192 7.625974 7.315949 5.500515

11 C 8.000907 6.787248 8.845923 8.268228 6.535701

12 C 9.343333 8.095623 10.114862 9.703679 7.914268

13 C 10.528166 9.332472 11.354908 10.754004 9.048943

14 H 2.098686 1.089318 2.552403 3.245897 2.164773

15 H 1.885612 3.212753 2.285841 0.972375 3.735840

16 H 3.480309 2.147032 4.495647 3.841582 1.091379

17 H 2.834893 2.158675 3.812669 2.988021 1.095202

18 H 2.851406 2.173210 4.054094 2.586825 1.090525

19 H 6.883669 5.698410 7.510761 7.445084 5.900936

20 H 7.163488 5.774171 7.905252 7.720875 5.618208

21 H 8.141145 6.896166 9.084101 8.299828 6.402277

22 H 7.944484 6.875273 8.785505 8.103683 6.700407

23 H 9.396885 8.203234 10.063024 9.847948 8.222915

24 H 9.588331 8.248590 10.353403 10.026422 8.003808

25 H 11.463440 10.243379 12.248617 11.750010 10.002132

26 H 10.684959 9.464907 11.591545 10.824414 9.006915

27 H 10.525085 9.436698 11.342419 10.673696 9.216858

6 7 8 9 10

6 S 0.000000

7 C 1.757853 0.000000

8 S 2.963537 1.789883 0.000000

9 S 3.054614 1.722494 3.090315 0.000000

10 C 4.330615 2.833047 1.840661 3.408861 0.000000

11 C 5.513542 4.197844 2.770983 4.919143 1.524859

12 C 6.773457 5.357104 4.171091 5.744708 2.532110

13 C 7.998926 6.693535 5.314242 7.219601 3.899335

14 H 2.422358 3.013001 4.471165 3.161716 5.787500

15 H 4.128116 5.685721 6.464314 6.704749 8.179801

16 H 3.012099 2.752953 3.214670 3.322060 4.746812

17 H 3.818189 4.210988 4.844794 4.705486 6.471261

18 H 3.047921 3.580158 3.762410 4.681256 5.566912

19 H 4.216319 2.864983 2.405931 3.365486 1.092556

20 H 4.777672 3.082833 2.420310 3.115507 1.090598

21 H 5.856928 4.543409 2.921088 5.280298 2.160000

22 H 5.449739 4.423692 2.954470 5.432120 2.157394

23 H 6.732098 5.383963 4.467210 5.700493 2.735450

24 H 7.092151 5.516629 4.463429 5.605861 2.769812

25 H 8.889789 7.528633 6.262278 7.892471 4.706957

26 H 8.286533 6.967425 5.442172 7.527876 4.236527

27 H 7.989497 6.870590 5.457915 7.602346 4.220526

11 12 13 14 15

11 C 0.000000

12 C 1.531566 0.000000

13 C 2.546370 1.527486 0.000000

14 H 7.126603 8.316763 9.649129 0.000000

15 H 9.123353 10.552281 11.588370 3.952767 0.000000

16 H 5.803986 7.119325 8.285235 2.479368 4.797437

17 H 7.503357 8.859138 9.989898 2.522038 3.823446

18 H 6.401069 7.864612 8.866643 3.079112 3.535826

19 H 2.170946 2.815853 4.218744 5.840919 8.244587

20 H 2.170109 2.771541 4.211893 5.812592 8.618161

21 H 1.096830 2.157280 2.788118 7.285137 9.190054

22 H 1.096114 2.159611 2.757045 7.338883 8.901164

23 H 2.157332 1.096678 2.157878 8.369240 10.652909

24 H 2.157895 1.096480 2.159115 8.357445 10.911409

25 H 3.500887 2.180391 1.094421 10.492999 12.584371

26 H 2.809851 2.179302 1.095179 9.823008 11.685555

27 H 2.820886 2.178662 1.095080 9.842162 11.458596

16 17 18 19 20

16 H 0.000000

17 H 1.767451 0.000000

18 H 1.770593 1.772915 0.000000

19 H 5.252883 6.907708 6.021759 0.000000

20 H 4.726196 6.485814 5.846195 1.767514 0.000000

21 H 5.624917 7.296317 6.201212 3.072996 2.534999

22 H 6.115397 7.720826 6.427146 2.497445 3.070567

23 H 7.481081 9.205558 8.228615 2.571867 3.048916

24 H 7.110527 8.875325 8.066949 3.171709 2.560143

25 H 9.203554 10.933228 9.875016 4.912104 4.882962

26 H 8.217180 9.890929 8.772661 4.787995 4.465848

27 H 8.554033 10.203475 8.938503 4.414331 4.767444

21 22 23 24 25

21 H 0.000000

22 H 1.758152 0.000000

23 H 3.060423 2.522950 0.000000

24 H 2.492514 3.062241 1.754593 0.000000

25 H 3.786095 3.771227 2.507173 2.498128 0.000000

26 H 2.605237 3.101084 3.077857 2.531065 1.765670

27 H 3.171051 2.584350 2.518102 3.077875 1.766160

26 27

26 H 0.000000

27 H 1.766797 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.12D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.118987 -0.411648 -0.217447

2 6 0 -2.856405 0.119498 0.401290

3 8 0 -4.875302 0.236192 -0.906312

4 8 0 -4.327899 -1.721728 0.039976

5 6 0 -2.440293 -0.527658 1.708875

6 16 0 -1.520902 -0.072470 -0.937996

7 6 0 -0.106325 0.643116 -0.178420

8 16 0 1.119854 -0.564302 0.313829

9 16 0 -0.033829 2.302369 0.278317

10 6 0 2.703032 0.298082 -0.057484

11 6 0 3.873816 -0.675143 0.027903

12 6 0 5.214322 0.020962 -0.225426

13 6 0 6.395535 -0.947122 -0.197837

14 1 0 -2.985656 1.194953 0.516636

15 1 0 -5.144486 -1.981013 -0.419881

16 1 0 -1.522889 -0.062794 2.074087

17 1 0 -3.215259 -0.384496 2.469402

18 1 0 -2.263732 -1.597663 1.594159

19 1 0 2.618169 0.721435 -1.061102

20 1 0 2.824967 1.120517 0.648305

21 1 0 3.894205 -1.148139 1.017294

22 1 0 3.738187 -1.481686 -0.701864

23 1 0 5.179265 0.529243 -1.196572

24 1 0 5.362687 0.805132 0.526460

25 1 0 7.343463 -0.427064 -0.367330

26 1 0 6.468814 -1.458612 0.767785

27 1 0 6.297731 -1.715609 -0.971829

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3259567 0.1910879 0.1795606

Leave Link 202 at Sat Aug 17 17:35:06 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1100.2553714800 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0547576173 Hartrees.

Nuclear repulsion after empirical dispersion term = 1100.2006138627 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2325

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.16D-09

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 95

GePol: Fraction of low-weight points (<1% of avg) = 4.09%

GePol: Cavity surface area = 309.296 Ang\*\*2

GePol: Cavity volume = 320.040 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0058176756 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1100.1947961872 Hartrees.

Leave Link 301 at Sat Aug 17 17:35:06 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.86D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:35:07 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:35:07 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999963 0.008641 0.000500 0.000174 Ang= 0.99 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7553 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.62922442022

Leave Link 401 at Sat Aug 17 17:35:07 2019, MaxMem= 1342177280 cpu: 7.5

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16216875.

Iteration 1 A\*A^-1 deviation from unit magnitude is 4.88D-15 for 2325.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.03D-15 for 2286 406.

Iteration 1 A^-1\*A deviation from unit magnitude is 4.66D-15 for 2325.

Iteration 1 A^-1\*A deviation from orthogonality is 4.50D-12 for 798 748.

E= -1658.67206461061

DIIS: error= 3.12D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67206461061 IErMin= 1 ErrMin= 3.12D-03

ErrMax= 3.12D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.07D-02 BMatP= 1.07D-02

IDIUse=3 WtCom= 9.69D-01 WtEn= 3.12D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.428 Goal= None Shift= 0.000

Gap= 0.482 Goal= None Shift= 0.000

GapD= 0.428 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=2.08D-04 MaxDP=5.15D-03 OVMax= 1.45D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.08D-04 CP: 1.00D+00

E= -1658.67681723119 Delta-E= -0.004752620578 Rises=F Damp=F

DIIS: error= 3.52D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67681723119 IErMin= 2 ErrMin= 3.52D-04

ErrMax= 3.52D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.59D-04 BMatP= 1.07D-02

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.52D-03

Coeff-Com: -0.696D-01 0.107D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.694D-01 0.107D+01

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.38D-05 MaxDP=8.75D-04 DE=-4.75D-03 OVMax= 2.08D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.95D-05 CP: 1.00D+00 1.08D+00

E= -1658.67685859491 Delta-E= -0.000041363723 Rises=F Damp=F

DIIS: error= 2.88D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67685859491 IErMin= 3 ErrMin= 2.88D-04

ErrMax= 2.88D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.73D-05 BMatP= 1.59D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 2.88D-03

Coeff-Com: -0.366D-01 0.494D+00 0.542D+00

Coeff-En: 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.365D-01 0.493D+00 0.544D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.14D-05 MaxDP=9.97D-04 DE=-4.14D-05 OVMax= 1.98D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.65D-05 CP: 1.00D+00 1.10D+00 5.55D-01

E= -1658.67687057911 Delta-E= -0.000011984197 Rises=F Damp=F

DIIS: error= 1.65D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67687057911 IErMin= 4 ErrMin= 1.65D-04

ErrMax= 1.65D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.39D-05 BMatP= 8.73D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.65D-03

Coeff-Com: -0.112D-01 0.140D+00 0.378D+00 0.493D+00

Coeff-En: 0.000D+00 0.000D+00 0.314D+00 0.686D+00

Coeff: -0.112D-01 0.140D+00 0.378D+00 0.493D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=9.23D-06 MaxDP=4.29D-04 DE=-1.20D-05 OVMax= 8.51D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.31D-06 CP: 1.00D+00 1.10D+00 7.15D-01 5.97D-01

E= -1658.67687811270 Delta-E= -0.000007533587 Rises=F Damp=F

DIIS: error= 2.70D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67687811270 IErMin= 5 ErrMin= 2.70D-05

ErrMax= 2.70D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.01D-06 BMatP= 3.39D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.288D-02 0.313D-01 0.147D+00 0.238D+00 0.587D+00

Coeff: -0.288D-02 0.313D-01 0.147D+00 0.238D+00 0.587D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.92D-06 MaxDP=9.66D-05 DE=-7.53D-06 OVMax= 1.79D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.33D-06 CP: 1.00D+00 1.10D+00 7.25D-01 6.68D-01 8.55D-01

E= -1658.67687830856 Delta-E= -0.000000195864 Rises=F Damp=F

DIIS: error= 1.54D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67687830856 IErMin= 6 ErrMin= 1.54D-05

ErrMax= 1.54D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.22D-07 BMatP= 1.01D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.624D-03-0.124D-01 0.925D-02 0.397D-01 0.344D+00 0.619D+00

Coeff: 0.624D-03-0.124D-01 0.925D-02 0.397D-01 0.344D+00 0.619D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=8.38D-07 MaxDP=3.57D-05 DE=-1.96D-07 OVMax= 1.15D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 6.52D-07 CP: 1.00D+00 1.10D+00 7.36D-01 6.87D-01 9.13D-01

CP: 8.99D-01

E= -1658.67687835515 Delta-E= -0.000000046593 Rises=F Damp=F

DIIS: error= 3.16D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67687835515 IErMin= 7 ErrMin= 3.16D-06

ErrMax= 3.16D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.71D-08 BMatP= 2.22D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.537D-03-0.858D-02-0.718D-02-0.276D-03 0.118D+00 0.294D+00

Coeff-Com: 0.604D+00

Coeff: 0.537D-03-0.858D-02-0.718D-02-0.276D-03 0.118D+00 0.294D+00

Coeff: 0.604D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.62D-07 MaxDP=1.30D-05 DE=-4.66D-08 OVMax= 5.41D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.69D-07 CP: 1.00D+00 1.10D+00 7.38D-01 6.88D-01 9.55D-01

CP: 9.98D-01 9.71D-01

E= -1658.67687835976 Delta-E= -0.000000004606 Rises=F Damp=F

DIIS: error= 2.57D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67687835976 IErMin= 8 ErrMin= 2.57D-06

ErrMax= 2.57D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.10D-09 BMatP= 1.71D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.167D-03-0.208D-02-0.598D-02-0.869D-02-0.640D-02 0.352D-01

Coeff-Com: 0.361D+00 0.627D+00

Coeff: 0.167D-03-0.208D-02-0.598D-02-0.869D-02-0.640D-02 0.352D-01

Coeff: 0.361D+00 0.627D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.22D-07 MaxDP=8.40D-06 DE=-4.61D-09 OVMax= 3.37D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.07D-07 CP: 1.00D+00 1.10D+00 7.38D-01 6.95D-01 9.70D-01

CP: 1.06D+00 1.15D+00 8.72D-01

E= -1658.67687836131 Delta-E= -0.000000001556 Rises=F Damp=F

DIIS: error= 1.22D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67687836131 IErMin= 9 ErrMin= 1.22D-06

ErrMax= 1.22D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.19D-09 BMatP= 5.10D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.225D-04 0.775D-03-0.207D-02-0.540D-02-0.319D-01-0.474D-01

Coeff-Com: 0.826D-01 0.384D+00 0.620D+00

Coeff: -0.225D-04 0.775D-03-0.207D-02-0.540D-02-0.319D-01-0.474D-01

Coeff: 0.826D-01 0.384D+00 0.620D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=9.84D-08 MaxDP=4.42D-06 DE=-1.56D-09 OVMax= 1.90D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 4.24D-08 CP: 1.00D+00 1.10D+00 7.39D-01 6.96D-01 9.76D-01

CP: 1.09D+00 1.23D+00 1.01D+00 8.95D-01

E= -1658.67687836166 Delta-E= -0.000000000343 Rises=F Damp=F

DIIS: error= 3.30D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67687836166 IErMin=10 ErrMin= 3.30D-07

ErrMax= 3.30D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.42D-10 BMatP= 1.19D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.401D-04 0.756D-03-0.305D-04-0.123D-02-0.149D-01-0.298D-01

Coeff-Com: -0.256D-01 0.767D-01 0.310D+00 0.684D+00

Coeff: -0.401D-04 0.756D-03-0.305D-04-0.123D-02-0.149D-01-0.298D-01

Coeff: -0.256D-01 0.767D-01 0.310D+00 0.684D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.52D-08 MaxDP=1.71D-06 DE=-3.43D-10 OVMax= 8.00D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.79D-08 CP: 1.00D+00 1.10D+00 7.39D-01 6.97D-01 9.78D-01

CP: 1.11D+00 1.26D+00 1.07D+00 9.98D-01 8.14D-01

E= -1658.67687836171 Delta-E= -0.000000000048 Rises=F Damp=F

DIIS: error= 9.24D-08 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67687836171 IErMin=11 ErrMin= 9.24D-08

ErrMax= 9.24D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.36D-11 BMatP= 1.42D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.118D-04 0.174D-03 0.207D-03 0.164D-03-0.158D-02-0.522D-02

Coeff-Com: -0.206D-01-0.215D-01 0.376D-01 0.267D+00 0.744D+00

Coeff: -0.118D-04 0.174D-03 0.207D-03 0.164D-03-0.158D-02-0.522D-02

Coeff: -0.206D-01-0.215D-01 0.376D-01 0.267D+00 0.744D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.44D-08 MaxDP=6.75D-07 DE=-4.82D-11 OVMax= 2.35D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 7.89D-09 CP: 1.00D+00 1.10D+00 7.39D-01 6.97D-01 9.79D-01

CP: 1.11D+00 1.27D+00 1.08D+00 1.05D+00 9.43D-01

CP: 9.12D-01

E= -1658.67687836174 Delta-E= -0.000000000037 Rises=F Damp=F

DIIS: error= 3.79D-08 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.67687836174 IErMin=12 ErrMin= 3.79D-08

ErrMax= 3.79D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.92D-12 BMatP= 1.36D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.643D-06-0.361D-04 0.102D-03 0.280D-03 0.160D-02 0.236D-02

Coeff-Com: -0.530D-02-0.221D-01-0.292D-01 0.212D-01 0.361D+00 0.670D+00

Coeff: 0.643D-06-0.361D-04 0.102D-03 0.280D-03 0.160D-02 0.236D-02

Coeff: -0.530D-02-0.221D-01-0.292D-01 0.212D-01 0.361D+00 0.670D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.59D-09 MaxDP=2.57D-07 DE=-3.68D-11 OVMax= 7.16D-07

Error on total polarization charges = 0.04183

SCF Done: E(UB3LYP) = -1658.67687836 A.U. after 12 cycles

NFock= 12 Conv=0.56D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7553 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655224300393D+03 PE=-6.143144442890D+03 EE= 1.729048467949D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.65

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7553, after 0.7500

Leave Link 502 at Sat Aug 17 17:35:32 2019, MaxMem= 1342177280 cpu: 290.8

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 340

Leave Link 701 at Sat Aug 17 17:35:33 2019, MaxMem= 1342177280 cpu: 10.2

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:35:33 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:35:36 2019, MaxMem= 1342177280 cpu: 36.1

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.30244182D+00-2.87759022D+00 5.73888639D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000231132 0.000153480 0.000651807

2 6 -0.000604235 -0.000036844 -0.000520231

3 8 0.000332932 -0.000334761 -0.000063192

4 8 -0.000011947 0.000338542 -0.000156872

5 6 0.000040154 -0.000114822 0.000109204

6 16 0.000065306 -0.000228844 0.000136151

7 6 -0.000012759 0.000521163 0.000422924

8 16 -0.000118637 -0.000218506 -0.000290243

9 16 -0.000045301 -0.000175219 -0.000229633

10 6 0.000092962 0.000076756 0.000119500

11 6 -0.000058040 -0.000051032 0.000015039

12 6 0.000093067 0.000069488 0.000008373

13 6 0.000003442 0.000053170 0.000036981

14 1 0.000250334 -0.000151619 0.000016680

15 1 0.000187918 0.000143697 0.000047805

16 1 -0.000092477 0.000085575 -0.000154883

17 1 0.000129282 -0.000064311 -0.000108092

18 1 0.000110511 0.000131821 -0.000047774

19 1 -0.000124173 -0.000194993 0.000205204

20 1 0.000108153 -0.000012637 -0.000141141

21 1 0.000062232 -0.000031866 -0.000156163

22 1 -0.000068104 0.000151192 0.000091838

23 1 0.000006062 -0.000050259 0.000105155

24 1 -0.000032429 -0.000069721 -0.000090125

25 1 -0.000116601 -0.000049412 -0.000001732

26 1 -0.000025382 0.000045640 -0.000129789

27 1 0.000058862 0.000014324 0.000123209

-------------------------------------------------------------------

Cartesian Forces: Max 0.000651807 RMS 0.000188075

Leave Link 716 at Sat Aug 17 17:35:36 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000778372 RMS 0.000167276

Search for a local minimum.

Step number 14 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .16728D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14

DE= -2.53D-05 DEPred=-2.28D-05 R= 1.11D+00

TightC=F SS= 1.41D+00 RLast= 1.25D-01 DXNew= 1.1892D-01 3.7358D-01

Trust test= 1.11D+00 RLast= 1.25D-01 DXMaxT set to 1.19D-01

ITU= 1 -1 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Eigenvalues --- 0.00084 0.00258 0.00330 0.00377 0.00463

Eigenvalues --- 0.00511 0.00593 0.00764 0.01633 0.01708

Eigenvalues --- 0.02337 0.03369 0.03556 0.03649 0.04579

Eigenvalues --- 0.04740 0.04837 0.04874 0.05067 0.05454

Eigenvalues --- 0.05472 0.05633 0.05720 0.05809 0.08215

Eigenvalues --- 0.08319 0.08408 0.11307 0.12102 0.12226

Eigenvalues --- 0.13815 0.14971 0.15983 0.16000 0.16022

Eigenvalues --- 0.16086 0.16092 0.16413 0.18085 0.18650

Eigenvalues --- 0.20027 0.21923 0.21986 0.23122 0.23382

Eigenvalues --- 0.24250 0.24914 0.25336 0.25592 0.26934

Eigenvalues --- 0.27961 0.29085 0.29437 0.29656 0.30240

Eigenvalues --- 0.30252 0.32395 0.33383 0.33862 0.33878

Eigenvalues --- 0.33893 0.33952 0.34011 0.34033 0.34093

Eigenvalues --- 0.34125 0.34256 0.34474 0.34546 0.34590

Eigenvalues --- 0.36078 0.39524 0.52635 0.56874 1.12138

En-DIIS/RFO-DIIS IScMMF= 0 using points: 14 13 12 11 10

RFO step: Lambda=-7.07248407D-06.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 2.80D-04 SmlDif= 1.00D-05

RMS Error= 0.4707623407D-03 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.06963 0.16560 -0.23620 -0.03076 0.03173

Iteration 1 RMS(Cart)= 0.02247399 RMS(Int)= 0.00022652

Iteration 2 RMS(Cart)= 0.00027814 RMS(Int)= 0.00000400

Iteration 3 RMS(Cart)= 0.00000005 RMS(Int)= 0.00000400

ITry= 1 IFail=0 DXMaxC= 5.97D-02 DCOld= 1.00D+10 DXMaxT= 1.19D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.84029 -0.00054 0.00010 0.00075 0.00086 2.84115

R2 2.28824 -0.00038 0.00005 0.00013 0.00018 2.28842

R3 2.55373 -0.00049 -0.00006 0.00040 0.00034 2.55407

R4 2.86700 -0.00013 -0.00010 -0.00040 -0.00051 2.86649

R5 3.59252 -0.00024 -0.00049 0.00006 -0.00043 3.59209

R6 2.05851 -0.00018 0.00004 0.00016 0.00021 2.05872

R7 1.83752 -0.00021 0.00003 0.00014 0.00017 1.83769

R8 2.06241 -0.00011 0.00009 0.00006 0.00015 2.06256

R9 2.06963 -0.00017 0.00002 0.00003 0.00005 2.06968

R10 2.06079 -0.00010 0.00000 0.00022 0.00022 2.06101

R11 3.32186 -0.00006 -0.00017 -0.00047 -0.00064 3.32122

R12 3.38239 0.00007 -0.00030 -0.00047 -0.00076 3.38163

R13 3.25504 -0.00026 0.00011 0.00049 0.00060 3.25564

R14 3.47834 -0.00003 0.00035 0.00081 0.00116 3.47951

R15 2.88157 -0.00013 -0.00005 -0.00005 -0.00010 2.88146

R16 2.06463 -0.00027 -0.00001 -0.00015 -0.00016 2.06448

R17 2.06093 -0.00010 0.00004 0.00017 0.00021 2.06115

R18 2.89424 0.00000 0.00000 0.00031 0.00031 2.89455

R19 2.07271 -0.00011 0.00001 0.00017 0.00018 2.07289

R20 2.07136 -0.00016 -0.00001 0.00004 0.00003 2.07138

R21 2.88653 -0.00011 -0.00004 -0.00016 -0.00020 2.88633

R22 2.07242 -0.00011 0.00001 0.00018 0.00020 2.07262

R23 2.07205 -0.00012 0.00000 0.00012 0.00012 2.07216

R24 2.06816 -0.00012 0.00000 0.00018 0.00018 2.06834

R25 2.06959 -0.00013 0.00001 0.00013 0.00013 2.06972

R26 2.06940 -0.00012 0.00001 0.00014 0.00015 2.06955

A1 2.17707 0.00011 -0.00010 -0.00102 -0.00114 2.17592

A2 1.97581 -0.00003 0.00023 0.00048 0.00070 1.97651

A3 2.12996 -0.00009 -0.00014 0.00024 0.00009 2.13004

A4 2.02023 0.00020 0.00040 0.00189 0.00229 2.02252

A5 1.83840 0.00032 -0.00040 -0.00102 -0.00142 1.83698

A6 1.86796 -0.00003 -0.00002 -0.00045 -0.00047 1.86749

A7 1.95134 -0.00054 -0.00010 -0.00112 -0.00121 1.95013

A8 1.94165 0.00001 0.00014 -0.00081 -0.00068 1.94098

A9 1.83138 0.00006 -0.00008 0.00151 0.00143 1.83281

A10 1.87364 -0.00019 -0.00031 0.00001 -0.00030 1.87334

A11 1.91481 -0.00027 0.00009 -0.00152 -0.00143 1.91338

A12 1.92694 0.00014 0.00009 0.00043 0.00053 1.92747

A13 1.95226 -0.00004 -0.00010 0.00084 0.00073 1.95299

A14 1.88257 0.00007 0.00002 0.00025 0.00027 1.88284

A15 1.89339 0.00008 -0.00012 -0.00005 -0.00017 1.89322

A16 1.89217 0.00002 0.00002 0.00005 0.00007 1.89224

A17 1.79240 -0.00078 -0.00028 -0.00032 -0.00060 1.79180

A18 1.97742 -0.00038 0.00058 0.00075 0.00134 1.97876

A19 2.14192 0.00001 -0.00018 -0.00041 -0.00057 2.14135

A20 2.15083 0.00036 -0.00039 -0.00010 -0.00048 2.15036

A21 1.79025 -0.00022 -0.00052 -0.00121 -0.00173 1.78852

A22 1.92844 0.00025 0.00030 0.00187 0.00217 1.93061

A23 1.87554 -0.00019 -0.00021 -0.00178 -0.00198 1.87355

A24 1.89540 0.00001 0.00011 0.00034 0.00045 1.89585

A25 1.93733 0.00001 -0.00011 -0.00008 -0.00019 1.93715

A26 1.93823 -0.00011 -0.00005 -0.00025 -0.00030 1.93793

A27 1.88699 0.00002 -0.00005 -0.00019 -0.00024 1.88675

A28 1.95268 -0.00017 -0.00017 -0.00106 -0.00123 1.95145

A29 1.91773 0.00013 0.00014 0.00078 0.00092 1.91865

A30 1.91489 -0.00003 -0.00009 -0.00003 -0.00012 1.91477

A31 1.90597 -0.00003 -0.00003 -0.00053 -0.00056 1.90541

A32 1.90987 0.00014 0.00006 0.00106 0.00112 1.91099

A33 1.86037 -0.00004 0.00010 -0.00016 -0.00006 1.86031

A34 1.96687 0.00008 0.00007 0.00074 0.00080 1.96767

A35 1.90619 -0.00002 -0.00008 0.00044 0.00035 1.90655

A36 1.90716 -0.00004 -0.00004 -0.00079 -0.00083 1.90633

A37 1.91182 0.00001 -0.00008 0.00039 0.00030 1.91212

A38 1.91371 -0.00004 0.00009 -0.00037 -0.00028 1.91343

A39 1.85469 0.00001 0.00006 -0.00047 -0.00041 1.85428

A40 1.94532 -0.00004 -0.00005 -0.00007 -0.00012 1.94521

A41 1.94299 -0.00001 0.00002 0.00003 0.00005 1.94304

A42 1.94221 0.00011 -0.00001 0.00063 0.00062 1.94282

A43 1.87604 0.00002 -0.00002 -0.00004 -0.00006 1.87598

A44 1.87692 -0.00003 0.00002 -0.00027 -0.00025 1.87668

A45 1.87696 -0.00006 0.00004 -0.00031 -0.00028 1.87669

D1 2.62145 0.00030 0.00371 0.02064 0.02435 2.64580

D2 -1.49673 -0.00002 0.00354 0.01967 0.02320 -1.47353

D3 0.44594 0.00018 0.00326 0.02074 0.02399 0.46993

D4 -0.54826 0.00007 0.00366 0.00884 0.01251 -0.53575

D5 1.61674 -0.00025 0.00349 0.00787 0.01136 1.62810

D6 -2.72377 -0.00005 0.00322 0.00894 0.01215 -2.71162

D7 -3.11052 0.00015 -0.00019 0.00861 0.00842 -3.10210

D8 0.00381 -0.00007 -0.00024 -0.00285 -0.00309 0.00072

D9 -3.13098 0.00002 -0.00054 0.00090 0.00036 -3.13062

D10 -1.05846 0.00002 -0.00040 0.00052 0.00012 -1.05834

D11 1.05024 0.00012 -0.00038 0.00144 0.00107 1.05130

D12 1.04720 -0.00013 -0.00022 0.00174 0.00151 1.04871

D13 3.11972 -0.00013 -0.00008 0.00136 0.00128 3.12099

D14 -1.05477 -0.00003 -0.00006 0.00228 0.00222 -1.05255

D15 -0.99405 0.00013 -0.00015 0.00108 0.00093 -0.99312

D16 1.07846 0.00014 -0.00001 0.00070 0.00069 1.07916

D17 -3.09602 0.00023 0.00001 0.00162 0.00164 -3.09439

D18 3.09075 0.00000 0.00310 0.00279 0.00588 3.09663

D19 -0.98452 0.00013 0.00325 0.00373 0.00699 -0.97753

D20 1.12221 -0.00012 0.00331 0.00309 0.00640 1.12861

D21 1.87536 -0.00005 0.00082 -0.00780 -0.00698 1.86839

D22 -1.09857 -0.00005 0.00047 -0.00929 -0.00882 -1.10739

D23 2.48420 0.00028 -0.00369 0.01278 0.00909 2.49329

D24 -0.82604 0.00023 -0.00331 0.01425 0.01094 -0.81510

D25 -2.93989 0.00003 0.00729 0.01977 0.02706 -2.91283

D26 -0.82385 0.00007 0.00720 0.01967 0.02687 -0.79698

D27 1.21346 0.00000 0.00709 0.01867 0.02576 1.23922

D28 -3.10510 0.00001 0.00094 0.01082 0.01176 -3.09334

D29 -0.98496 -0.00004 0.00089 0.00997 0.01086 -0.97410

D30 1.05497 -0.00003 0.00103 0.01021 0.01125 1.06621

D31 1.09913 0.00008 0.00107 0.01188 0.01295 1.11208

D32 -3.06391 0.00002 0.00102 0.01103 0.01205 -3.05187

D33 -1.02399 0.00003 0.00117 0.01127 0.01244 -1.01155

D34 -1.00066 0.00012 0.00125 0.01233 0.01358 -0.98708

D35 1.11948 0.00006 0.00119 0.01148 0.01268 1.13216

D36 -3.12377 0.00008 0.00134 0.01173 0.01307 -3.11071

D37 -3.10280 -0.00002 0.00150 -0.00276 -0.00126 -3.10406

D38 -0.97380 0.00003 0.00138 -0.00146 -0.00008 -0.97387

D39 1.04827 0.00001 0.00138 -0.00222 -0.00084 1.04743

D40 1.05348 -0.00005 0.00146 -0.00267 -0.00121 1.05226

D41 -3.10071 0.00000 0.00133 -0.00137 -0.00004 -3.10074

D42 -1.07864 -0.00003 0.00133 -0.00213 -0.00080 -1.07943

D43 -0.97679 -0.00007 0.00132 -0.00277 -0.00145 -0.97825

D44 1.15221 -0.00002 0.00120 -0.00147 -0.00028 1.15193

D45 -3.10891 -0.00005 0.00119 -0.00223 -0.00104 -3.10994

D46 -3.12804 0.00003 0.00060 0.00537 0.00598 -3.12206

D47 -1.03352 0.00002 0.00056 0.00529 0.00586 -1.02767

D48 1.06005 0.00001 0.00062 0.00534 0.00595 1.06601

D49 1.02933 -0.00001 0.00073 0.00404 0.00477 1.03409

D50 3.12384 -0.00002 0.00069 0.00396 0.00464 3.12848

D51 -1.06577 -0.00003 0.00074 0.00401 0.00474 -1.06103

D52 -0.99962 0.00000 0.00066 0.00460 0.00526 -0.99437

D53 1.09489 0.00000 0.00061 0.00452 0.00513 1.10002

D54 -3.09472 -0.00001 0.00067 0.00457 0.00523 -3.08949

Item Value Threshold Converged?

Maximum Force 0.000778 0.000450 NO

RMS Force 0.000167 0.000300 YES

Maximum Displacement 0.059708 0.001800 NO

RMS Displacement 0.022478 0.001200 NO

Predicted change in Energy=-1.328067D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:35:36 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.092748 -0.412434 -0.266142

2 6 0 -2.840425 0.040999 0.431363

3 8 0 -4.837186 0.313779 -0.886545

4 8 0 -4.298377 -1.745487 -0.180154

5 6 0 -2.424831 -0.773282 1.641798

6 16 0 -1.494083 0.044695 -0.910499

7 6 0 -0.090138 0.653256 -0.045948

8 16 0 1.135171 -0.605874 0.293828

9 16 0 -0.027223 2.237368 0.628372

10 6 0 2.717600 0.309631 0.074583

11 6 0 3.893024 -0.659114 0.004283

12 6 0 5.231289 0.077225 -0.109922

13 6 0 6.419779 -0.874015 -0.234550

14 1 0 -2.982489 1.089341 0.691457

15 1 0 -5.103710 -1.947683 -0.686360

16 1 0 -1.515455 -0.351028 2.073093

17 1 0 -3.205911 -0.743868 2.408982

18 1 0 -2.233572 -1.815759 1.384582

19 1 0 2.633136 0.889997 -0.847122

20 1 0 2.834337 1.007252 0.904853

21 1 0 3.907076 -1.295444 0.897663

22 1 0 3.769433 -1.328555 -0.854827

23 1 0 5.203081 0.745374 -0.979239

24 1 0 5.365168 0.721070 0.767543

25 1 0 7.365802 -0.326871 -0.294909

26 1 0 6.483318 -1.547141 0.627096

27 1 0 6.340093 -1.495067 -1.133056

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.503472 0.000000

3 O 1.210980 2.407975 0.000000

4 O 1.351558 2.385604 2.242740 0.000000

5 C 2.559764 1.516879 3.659737 2.788344 0.000000

6 S 2.716104 1.900853 3.354000 3.406203 2.837181

7 C 4.147899 2.857755 4.832837 4.845746 3.214699

8 S 5.261380 4.030226 6.156954 5.571967 3.810337

9 S 4.934582 3.574487 5.397306 5.895727 3.979895

10 C 6.856989 5.575938 7.615679 7.315212 5.483927

11 C 7.994156 6.783206 8.829307 8.265184 6.527617

12 C 9.338192 8.089923 10.101153 9.702666 7.899877

13 C 10.522702 9.329097 11.338219 10.753664 9.042011

14 H 2.098809 1.089428 2.555677 3.244613 2.164138

15 H 1.885634 3.213506 2.285896 0.972466 3.738439

16 H 3.481125 2.145812 4.498369 3.842693 1.091458

17 H 2.837713 2.158836 3.826247 2.983344 1.095227

18 H 2.854951 2.173579 4.058541 2.591670 1.090642

19 H 6.875418 5.684645 7.492616 7.445568 5.877436

20 H 7.167373 5.775877 7.908367 7.722073 5.601093

21 H 8.132117 6.894366 9.068358 8.288165 6.396831

22 H 7.937235 6.871694 8.761972 8.106698 6.701520

23 H 9.394757 8.196580 10.049966 9.854979 8.207386

24 H 9.581519 8.240587 10.343593 10.018290 7.980069

25 H 11.458906 10.238646 12.234108 11.750690 9.990327

26 H 10.674203 9.460057 11.571860 10.813692 8.999089

27 H 10.524628 9.438687 11.325381 10.683996 9.221968

6 7 8 9 10

6 S 0.000000

7 C 1.757514 0.000000

8 S 2.964223 1.789479 0.000000

9 S 3.054115 1.722811 3.089838 0.000000

10 C 4.333456 2.831253 1.841276 3.399545 0.000000

11 C 5.509364 4.194093 2.773522 4.914003 1.524805

12 C 6.772932 5.352895 4.172268 5.732647 2.531144

13 C 7.995633 6.689331 5.317722 7.210352 3.899066

14 H 2.423407 3.016559 4.470680 3.171048 5.786146

15 H 4.129070 5.684269 6.456381 6.709239 8.176025

16 H 3.009796 2.744166 3.202584 3.316903 4.727501

17 H 3.817216 4.205553 4.830933 4.707696 6.453469

18 H 3.045575 3.568860 3.741925 4.676288 5.545042

19 H 4.213370 2.848534 2.404848 3.327161 1.092473

20 H 4.791371 3.095463 2.421300 3.127004 1.090711

21 H 5.851320 4.545939 2.919518 5.294525 2.160691

22 H 5.439992 4.413405 2.963277 5.415744 2.157269

23 H 6.734068 5.375656 4.471516 5.671555 2.734598

24 H 7.093845 5.516043 4.458482 5.603250 2.767507

25 H 8.889014 7.524206 6.264601 7.879378 4.706108

26 H 8.278712 6.964558 5.440564 7.530582 4.234798

27 H 7.987159 6.866219 5.469724 7.587912 4.223480

11 12 13 14 15

11 C 0.000000

12 C 1.531728 0.000000

13 C 2.547099 1.527382 0.000000

14 H 7.127550 8.314610 9.649606 0.000000

15 H 9.114747 10.547262 11.582215 3.952401 0.000000

16 H 5.798839 7.104048 8.280499 2.477049 4.799944

17 H 7.495641 8.843383 9.982941 2.521996 3.825173

18 H 6.385784 7.844813 8.853754 3.079107 3.541736

19 H 2.170703 2.820366 4.222043 5.825994 8.242394

20 H 2.169935 2.764072 4.206281 5.821318 8.618364

21 H 1.096924 2.157078 2.788043 7.293547 9.172176

22 H 1.096128 2.160585 2.759653 7.336597 8.896312

23 H 2.157811 1.096782 2.158086 8.361405 10.656842

24 H 2.157471 1.096541 2.158863 8.356123 10.901077

25 H 3.501442 2.180289 1.094518 10.491220 12.580501

26 H 2.808223 2.179298 1.095250 9.826326 11.668112

27 H 2.824979 2.179072 1.095157 9.844722 11.461459

16 17 18 19 20

16 H 0.000000

17 H 1.767707 0.000000

18 H 1.770643 1.773073 0.000000

19 H 5.222892 6.882311 5.998872 0.000000

20 H 4.704296 6.466330 5.820931 1.767384 0.000000

21 H 5.628268 7.292662 6.181859 3.073004 2.540321

22 H 6.120319 7.723324 6.425604 2.492630 3.070321

23 H 7.460398 9.187439 8.212847 2.577399 3.037981

24 H 7.084972 8.848942 8.034743 3.177999 2.550659

25 H 9.191558 10.919984 9.858269 4.917707 4.873755

26 H 8.215958 9.884409 8.753863 4.789245 4.462862

27 H 8.561416 10.209629 8.941425 4.417219 4.764976

21 22 23 24 25

21 H 0.000000

22 H 1.758199 0.000000

23 H 3.060609 2.524284 0.000000

24 H 2.491845 3.062583 1.754453 0.000000

25 H 3.784594 3.775017 2.509060 2.495901 0.000000

26 H 2.602610 3.099847 3.078140 2.532739 1.765767

27 H 3.175412 2.591029 2.517148 3.077989 1.766140

26 27

26 H 0.000000

27 H 1.766737 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.56D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.117862 -0.411600 -0.216171

2 6 0 -2.855766 0.122196 0.402379

3 8 0 -4.863592 0.229810 -0.922538

4 8 0 -4.331393 -1.719103 0.051312

5 6 0 -2.433619 -0.524051 1.708165

6 16 0 -1.522729 -0.066274 -0.939535

7 6 0 -0.106355 0.642632 -0.177831

8 16 0 1.113940 -0.568523 0.318376

9 16 0 -0.026378 2.302873 0.275245

10 6 0 2.700115 0.296447 -0.036834

11 6 0 3.868394 -0.682097 0.014222

12 6 0 5.210280 0.021489 -0.210496

13 6 0 6.391203 -0.947165 -0.215753

14 1 0 -2.988363 1.197173 0.519410

15 1 0 -5.142992 -1.981606 -0.415689

16 1 0 -1.517276 -0.054474 2.070233

17 1 0 -3.206884 -0.384971 2.471212

18 1 0 -2.251764 -1.593213 1.592755

19 1 0 2.610383 0.747406 -1.027834

20 1 0 2.829620 1.099057 0.690282

21 1 0 3.887072 -1.191785 0.985361

22 1 0 3.731937 -1.460636 -0.745221

23 1 0 5.177894 0.566069 -1.161976

24 1 0 5.357037 0.777070 0.570506

25 1 0 7.340162 -0.420663 -0.358026

26 1 0 6.458810 -1.497991 0.728489

27 1 0 6.298578 -1.683436 -1.021168

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3237711 0.1913730 0.1798421

Leave Link 202 at Sat Aug 17 17:35:37 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1100.5933868571 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0547996627 Hartrees.

Nuclear repulsion after empirical dispersion term = 1100.5385871944 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2333

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.82D-08

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 103

GePol: Fraction of low-weight points (<1% of avg) = 4.41%

GePol: Cavity surface area = 309.224 Ang\*\*2

GePol: Cavity volume = 319.964 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0058491802 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1100.5327380142 Hartrees.

Leave Link 301 at Sat Aug 17 17:35:37 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.86D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:35:37 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:35:37 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999999 -0.001046 -0.000049 0.000266 Ang= -0.12 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7553 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.62927678810

Leave Link 401 at Sat Aug 17 17:35:38 2019, MaxMem= 1342177280 cpu: 7.5

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16328667.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.22D-15 for 2326.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.97D-15 for 2295 2035.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.88D-15 for 2326.

Iteration 1 A^-1\*A deviation from orthogonality is 2.19D-10 for 1327 1167.

Iteration 2 A\*A^-1 deviation from unit magnitude is 7.99D-15 for 386.

Iteration 2 A\*A^-1 deviation from orthogonality is 5.49D-15 for 892 772.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.33D-15 for 1936.

Iteration 2 A^-1\*A deviation from orthogonality is 9.56D-16 for 2301 64.

E= -1658.67538155687

DIIS: error= 1.74D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67538155687 IErMin= 1 ErrMin= 1.74D-03

ErrMax= 1.74D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.25D-03 BMatP= 3.25D-03

IDIUse=3 WtCom= 9.83D-01 WtEn= 1.74D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.428 Goal= None Shift= 0.000

Gap= 0.483 Goal= None Shift= 0.000

GapD= 0.428 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=1.08D-04 MaxDP=2.39D-03 OVMax= 9.61D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.08D-04 CP: 1.00D+00

E= -1658.67685958060 Delta-E= -0.001478023727 Rises=F Damp=F

DIIS: error= 1.85D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67685958060 IErMin= 2 ErrMin= 1.85D-04

ErrMax= 1.85D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.93D-05 BMatP= 3.25D-03

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.85D-03

Coeff-Com: -0.732D-01 0.107D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.730D-01 0.107D+01

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.71D-05 MaxDP=3.26D-04 DE=-1.48D-03 OVMax= 1.08D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.26D-05 CP: 1.00D+00 1.11D+00

E= -1658.67687526622 Delta-E= -0.000015685624 Rises=F Damp=F

DIIS: error= 8.93D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67687526622 IErMin= 3 ErrMin= 8.93D-05

ErrMax= 8.93D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.22D-06 BMatP= 3.93D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.292D-01 0.379D+00 0.650D+00

Coeff: -0.292D-01 0.379D+00 0.650D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.86D-06 MaxDP=2.74D-04 DE=-1.57D-05 OVMax= 5.45D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 6.18D-06 CP: 1.00D+00 1.12D+00 7.86D-01

E= -1658.67687614760 Delta-E= -0.000000881378 Rises=F Damp=F

DIIS: error= 7.44D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67687614760 IErMin= 4 ErrMin= 7.44D-05

ErrMax= 7.44D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.47D-06 BMatP= 9.22D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.989D-02 0.117D+00 0.432D+00 0.461D+00

Coeff: -0.989D-02 0.117D+00 0.432D+00 0.461D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.61D-06 MaxDP=1.54D-04 DE=-8.81D-07 OVMax= 3.02D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.02D-06 CP: 1.00D+00 1.12D+00 9.07D-01 5.86D-01

E= -1658.67687729741 Delta-E= -0.000001149811 Rises=F Damp=F

DIIS: error= 1.37D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67687729741 IErMin= 5 ErrMin= 1.37D-05

ErrMax= 1.37D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.59D-07 BMatP= 5.47D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.246D-02 0.235D-01 0.168D+00 0.244D+00 0.567D+00

Coeff: -0.246D-02 0.235D-01 0.168D+00 0.244D+00 0.567D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=9.92D-07 MaxDP=3.48D-05 DE=-1.15D-06 OVMax= 6.96D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 6.67D-07 CP: 1.00D+00 1.12D+00 9.22D-01 6.49D-01 7.07D-01

E= -1658.67687734780 Delta-E= -0.000000050388 Rises=F Damp=F

DIIS: error= 5.62D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67687734780 IErMin= 6 ErrMin= 5.62D-06

ErrMax= 5.62D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.80D-08 BMatP= 2.59D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.459D-03-0.966D-02 0.171D-01 0.568D-01 0.334D+00 0.601D+00

Coeff: 0.459D-03-0.966D-02 0.171D-01 0.568D-01 0.334D+00 0.601D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.27D-07 MaxDP=2.18D-05 DE=-5.04D-08 OVMax= 4.92D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.76D-07 CP: 1.00D+00 1.12D+00 9.32D-01 6.63D-01 8.20D-01

CP: 7.57D-01

E= -1658.67687735891 Delta-E= -0.000000011112 Rises=F Damp=F

DIIS: error= 1.42D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67687735891 IErMin= 7 ErrMin= 1.42D-06

ErrMax= 1.42D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.50D-09 BMatP= 4.80D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.396D-03-0.623D-02-0.444D-02 0.805D-02 0.108D+00 0.286D+00

Coeff-Com: 0.609D+00

Coeff: 0.396D-03-0.623D-02-0.444D-02 0.805D-02 0.108D+00 0.286D+00

Coeff: 0.609D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.50D-07 MaxDP=4.89D-06 DE=-1.11D-08 OVMax= 1.44D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.14D-07 CP: 1.00D+00 1.12D+00 9.34D-01 6.64D-01 8.56D-01

CP: 8.36D-01 9.45D-01

E= -1658.67687735975 Delta-E= -0.000000000836 Rises=F Damp=F

DIIS: error= 5.63D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67687735975 IErMin= 8 ErrMin= 5.63D-07

ErrMax= 5.63D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.49D-10 BMatP= 3.50D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.107D-03-0.120D-02-0.528D-02-0.639D-02-0.103D-01 0.341D-01

Coeff-Com: 0.324D+00 0.665D+00

Coeff: 0.107D-03-0.120D-02-0.528D-02-0.639D-02-0.103D-01 0.341D-01

Coeff: 0.324D+00 0.665D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=7.59D-08 MaxDP=2.69D-06 DE=-8.36D-10 OVMax= 7.63D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 4.30D-08 CP: 1.00D+00 1.12D+00 9.35D-01 6.68D-01 8.63D-01

CP: 8.86D-01 1.10D+00 9.19D-01

E= -1658.67687735996 Delta-E= -0.000000000215 Rises=F Damp=F

DIIS: error= 4.58D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67687735996 IErMin= 9 ErrMin= 4.58D-07

ErrMax= 4.58D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.94D-10 BMatP= 7.49D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.122D-04 0.511D-03-0.230D-02-0.535D-02-0.280D-01-0.344D-01

Coeff-Com: 0.807D-01 0.395D+00 0.593D+00

Coeff: -0.122D-04 0.511D-03-0.230D-02-0.535D-02-0.280D-01-0.344D-01

Coeff: 0.807D-01 0.395D+00 0.593D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.09D-08 MaxDP=1.36D-06 DE=-2.15D-10 OVMax= 5.25D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.91D-08 CP: 1.00D+00 1.12D+00 9.36D-01 6.68D-01 8.71D-01

CP: 8.95D-01 1.18D+00 1.08D+00 7.96D-01

E= -1658.67687736003 Delta-E= -0.000000000069 Rises=F Damp=F

DIIS: error= 1.93D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67687736003 IErMin=10 ErrMin= 1.93D-07

ErrMax= 1.93D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.89D-11 BMatP= 1.94D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.304D-04 0.566D-03-0.235D-03-0.180D-02-0.146D-01-0.291D-01

Coeff-Com: -0.330D-01 0.719D-01 0.353D+00 0.653D+00

Coeff: -0.304D-04 0.566D-03-0.235D-03-0.180D-02-0.146D-01-0.291D-01

Coeff: -0.330D-01 0.719D-01 0.353D+00 0.653D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.73D-08 MaxDP=5.93D-07 DE=-6.87D-11 OVMax= 1.76D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 8.26D-09 CP: 1.00D+00 1.12D+00 9.36D-01 6.68D-01 8.72D-01

CP: 9.05D-01 1.21D+00 1.13D+00 9.26D-01 8.20D-01

E= -1658.67687736003 Delta-E= 0.000000000001 Rises=F Damp=F

DIIS: error= 5.29D-08 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=10 EnMin= -1658.67687736003 IErMin=11 ErrMin= 5.29D-08

ErrMax= 5.29D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.28D-12 BMatP= 3.89D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.122D-04 0.188D-03 0.179D-03-0.150D-03-0.302D-02-0.882D-02

Coeff-Com: -0.261D-01-0.182D-01 0.886D-01 0.326D+00 0.641D+00

Coeff: -0.122D-04 0.188D-03 0.179D-03-0.150D-03-0.302D-02-0.882D-02

Coeff: -0.261D-01-0.182D-01 0.886D-01 0.326D+00 0.641D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.31D-09 MaxDP=2.15D-07 DE= 9.09D-13 OVMax= 7.05D-07

Error on total polarization charges = 0.04180

SCF Done: E(UB3LYP) = -1658.67687736 A.U. after 11 cycles

NFock= 11 Conv=0.63D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655222341366D+03 PE=-6.143823048777D+03 EE= 1.729391092036D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.67

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:36:02 2019, MaxMem= 1342177280 cpu: 277.0

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 340

Leave Link 701 at Sat Aug 17 17:36:02 2019, MaxMem= 1342177280 cpu: 10.3

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:36:03 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:36:06 2019, MaxMem= 1342177280 cpu: 36.0

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.30172681D+00-2.87423290D+00 5.90908415D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000756712 -0.000019501 -0.000473669

2 6 -0.001330781 -0.000124739 -0.000212472

3 8 -0.000013523 -0.000359622 0.000451570

4 8 -0.000201032 0.000525195 0.000157451

5 6 0.000047968 -0.000123585 0.000236821

6 16 0.000305029 -0.000197392 0.000080514

7 6 -0.000171094 0.000780559 0.000392605

8 16 0.000193460 -0.000174367 -0.000423874

9 16 -0.000088932 -0.000279614 -0.000238380

10 6 0.000027606 -0.000015769 0.000038266

11 6 -0.000074549 -0.000026150 0.000124788

12 6 0.000057920 0.000090659 -0.000041480

13 6 0.000121403 0.000002134 0.000081124

14 1 0.000352929 -0.000120832 -0.000054515

15 1 0.000224142 0.000162514 0.000123340

16 1 -0.000178445 -0.000019143 -0.000088673

17 1 0.000158902 -0.000054888 -0.000130883

18 1 0.000064904 0.000194719 -0.000065786

19 1 -0.000086892 -0.000189194 0.000267083

20 1 0.000033271 -0.000045728 -0.000224680

21 1 0.000038191 0.000009977 -0.000171663

22 1 -0.000023787 0.000140451 0.000157667

23 1 0.000033946 -0.000122559 0.000109403

24 1 -0.000056825 -0.000063824 -0.000145750

25 1 -0.000176441 -0.000066769 -0.000027245

26 1 -0.000044237 0.000110447 -0.000132268

27 1 0.000030159 -0.000012979 0.000210705

-------------------------------------------------------------------

Cartesian Forces: Max 0.001330781 RMS 0.000261483

Leave Link 716 at Sat Aug 17 17:36:06 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000854404 RMS 0.000178084

Search for a local minimum.

Step number 15 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .17808D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15

DE= 1.00D-06 DEPred=-1.33D-05 R=-7.54D-02

Trust test=-7.54D-02 RLast= 8.05D-02 DXMaxT set to 5.95D-02

ITU= -1 1 -1 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Eigenvalues --- 0.00192 0.00238 0.00318 0.00373 0.00481

Eigenvalues --- 0.00503 0.00629 0.00926 0.01521 0.02314

Eigenvalues --- 0.02499 0.02945 0.03513 0.03620 0.04576

Eigenvalues --- 0.04738 0.04841 0.04949 0.04993 0.05454

Eigenvalues --- 0.05473 0.05604 0.05660 0.05806 0.08205

Eigenvalues --- 0.08331 0.08434 0.11320 0.12143 0.12225

Eigenvalues --- 0.13872 0.15199 0.16000 0.16026 0.16030

Eigenvalues --- 0.16065 0.16137 0.16389 0.18359 0.18758

Eigenvalues --- 0.19648 0.21917 0.21976 0.22722 0.23527

Eigenvalues --- 0.24360 0.25044 0.25219 0.25573 0.26673

Eigenvalues --- 0.27717 0.28764 0.29179 0.29477 0.29770

Eigenvalues --- 0.30429 0.31154 0.33515 0.33688 0.33875

Eigenvalues --- 0.33880 0.33898 0.33952 0.34022 0.34035

Eigenvalues --- 0.34097 0.34175 0.34344 0.34481 0.34550

Eigenvalues --- 0.34623 0.39149 0.52645 0.57291 1.31971

En-DIIS/RFO-DIIS IScMMF= 0 using points: 15 14 13 12 11

RFO step: Lambda=-8.71681833D-06.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 4.70D-05 SmlDif= 1.00D-05

RMS Error= 0.5274208606D-03 NUsed= 5 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.53487 0.41449 -0.32422 0.21761 0.15724

Iteration 1 RMS(Cart)= 0.03400152 RMS(Int)= 0.00029399

Iteration 2 RMS(Cart)= 0.00100997 RMS(Int)= 0.00000066

Iteration 3 RMS(Cart)= 0.00000042 RMS(Int)= 0.00000065

ITry= 1 IFail=0 DXMaxC= 1.38D-01 DCOld= 1.00D+10 DXMaxT= 5.95D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.84115 -0.00085 -0.00043 -0.00067 -0.00110 2.84005

R2 2.28842 -0.00044 -0.00087 -0.00036 -0.00122 2.28720

R3 2.55407 -0.00067 -0.00019 -0.00033 -0.00051 2.55356

R4 2.86649 0.00001 0.00021 -0.00024 -0.00003 2.86645

R5 3.59209 0.00005 0.00048 -0.00009 0.00038 3.59247

R6 2.05872 -0.00018 -0.00035 -0.00022 -0.00057 2.05815

R7 1.83769 -0.00028 -0.00032 -0.00026 -0.00058 1.83711

R8 2.06256 -0.00019 -0.00033 -0.00020 -0.00054 2.06202

R9 2.06968 -0.00021 -0.00018 -0.00026 -0.00043 2.06925

R10 2.06101 -0.00015 -0.00027 -0.00011 -0.00038 2.06063

R11 3.32122 -0.00011 0.00058 -0.00057 0.00002 3.32124

R12 3.38163 0.00024 0.00068 0.00023 0.00091 3.38254

R13 3.25564 -0.00035 -0.00057 -0.00012 -0.00069 3.25495

R14 3.47951 -0.00021 -0.00087 -0.00036 -0.00123 3.47828

R15 2.88146 -0.00014 -0.00001 -0.00027 -0.00028 2.88118

R16 2.06448 -0.00032 -0.00011 -0.00044 -0.00055 2.06393

R17 2.06115 -0.00019 -0.00030 -0.00023 -0.00053 2.06062

R18 2.89455 -0.00005 -0.00025 -0.00002 -0.00027 2.89428

R19 2.07289 -0.00015 -0.00022 -0.00014 -0.00036 2.07253

R20 2.07138 -0.00020 -0.00014 -0.00022 -0.00036 2.07102

R21 2.88633 -0.00009 0.00002 -0.00028 -0.00025 2.88608

R22 2.07262 -0.00016 -0.00025 -0.00014 -0.00039 2.07223

R23 2.07216 -0.00016 -0.00018 -0.00015 -0.00033 2.07183

R24 2.06834 -0.00018 -0.00021 -0.00016 -0.00037 2.06797

R25 2.06972 -0.00018 -0.00020 -0.00020 -0.00040 2.06933

R26 2.06955 -0.00016 -0.00020 -0.00016 -0.00036 2.06918

A1 2.17592 0.00030 0.00084 0.00012 0.00096 2.17689

A2 1.97651 -0.00016 -0.00089 -0.00031 -0.00120 1.97531

A3 2.13004 -0.00012 0.00021 0.00024 0.00045 2.13049

A4 2.02252 -0.00007 -0.00139 0.00103 -0.00037 2.02216

A5 1.83698 0.00032 0.00130 0.00002 0.00132 1.83830

A6 1.86749 0.00007 0.00056 0.00068 0.00124 1.86873

A7 1.95013 -0.00033 0.00029 -0.00166 -0.00137 1.94876

A8 1.94098 0.00008 -0.00003 -0.00035 -0.00038 1.94060

A9 1.83281 -0.00005 -0.00060 0.00032 -0.00029 1.83252

A10 1.87334 -0.00021 0.00089 -0.00074 0.00015 1.87349

A11 1.91338 -0.00005 0.00051 -0.00105 -0.00054 1.91284

A12 1.92747 0.00013 -0.00007 0.00061 0.00054 1.92801

A13 1.95299 -0.00015 -0.00009 0.00003 -0.00006 1.95294

A14 1.88284 -0.00001 -0.00028 0.00023 -0.00005 1.88280

A15 1.89322 0.00005 0.00008 -0.00003 0.00005 1.89327

A16 1.89224 0.00004 -0.00017 0.00022 0.00006 1.89229

A17 1.79180 -0.00037 0.00049 -0.00083 -0.00033 1.79147

A18 1.97876 -0.00041 -0.00130 -0.00162 -0.00292 1.97584

A19 2.14135 0.00002 0.00054 -0.00024 0.00030 2.14165

A20 2.15036 0.00037 0.00051 0.00080 0.00131 2.15166

A21 1.78852 0.00028 0.00163 0.00021 0.00184 1.79036

A22 1.93061 0.00001 -0.00128 0.00040 -0.00087 1.92973

A23 1.87355 -0.00013 0.00099 -0.00088 0.00010 1.87366

A24 1.89585 0.00009 -0.00013 0.00017 0.00004 1.89589

A25 1.93715 0.00020 0.00025 0.00047 0.00071 1.93786

A26 1.93793 -0.00014 0.00011 -0.00012 -0.00001 1.93792

A27 1.88675 -0.00004 0.00012 -0.00008 0.00004 1.88679

A28 1.95145 0.00000 0.00088 -0.00039 0.00049 1.95194

A29 1.91865 0.00000 -0.00062 0.00034 -0.00028 1.91837

A30 1.91477 0.00002 0.00016 0.00003 0.00020 1.91497

A31 1.90541 0.00000 0.00023 -0.00024 -0.00001 1.90539

A32 1.91099 0.00001 -0.00049 0.00057 0.00008 1.91107

A33 1.86031 -0.00002 -0.00021 -0.00030 -0.00052 1.85980

A34 1.96767 0.00001 -0.00042 0.00026 -0.00017 1.96750

A35 1.90655 -0.00002 -0.00007 0.00041 0.00035 1.90689

A36 1.90633 0.00001 0.00051 -0.00044 0.00006 1.90639

A37 1.91212 0.00004 0.00000 0.00044 0.00044 1.91256

A38 1.91343 -0.00004 0.00002 -0.00038 -0.00036 1.91307

A39 1.85428 0.00000 -0.00001 -0.00032 -0.00033 1.85395

A40 1.94521 -0.00004 0.00024 -0.00010 0.00014 1.94535

A41 1.94304 -0.00005 0.00004 -0.00008 -0.00004 1.94300

A42 1.94282 0.00011 -0.00017 0.00056 0.00039 1.94321

A43 1.87598 0.00005 -0.00013 0.00012 -0.00001 1.87598

A44 1.87668 -0.00001 -0.00003 -0.00011 -0.00014 1.87654

A45 1.87669 -0.00006 0.00004 -0.00042 -0.00038 1.87631

D1 2.64580 -0.00004 -0.01671 0.00777 -0.00894 2.63686

D2 -1.47353 -0.00027 -0.01625 0.00632 -0.00993 -1.48347

D3 0.46993 -0.00015 -0.01613 0.00696 -0.00917 0.46076

D4 -0.53575 0.00029 -0.01139 0.00910 -0.00229 -0.53805

D5 1.62810 0.00007 -0.01093 0.00764 -0.00329 1.62481

D6 -2.71162 0.00019 -0.01081 0.00829 -0.00253 -2.71415

D7 -3.10210 -0.00016 -0.00350 0.00077 -0.00273 -3.10483

D8 0.00072 0.00017 0.00168 0.00205 0.00373 0.00445

D9 -3.13062 0.00001 0.00078 0.00289 0.00368 -3.12694

D10 -1.05834 0.00004 0.00072 0.00290 0.00361 -1.05472

D11 1.05130 0.00008 0.00039 0.00363 0.00402 1.05532

D12 1.04871 -0.00011 -0.00014 0.00342 0.00328 1.05199

D13 3.12099 -0.00007 -0.00021 0.00343 0.00321 3.12421

D14 -1.05255 -0.00004 -0.00053 0.00415 0.00362 -1.04893

D15 -0.99312 0.00011 0.00044 0.00431 0.00476 -0.98837

D16 1.07916 0.00015 0.00038 0.00432 0.00469 1.08385

D17 -3.09439 0.00019 0.00005 0.00505 0.00510 -3.08929

D18 3.09663 -0.00001 0.00279 0.01231 0.01510 3.11173

D19 -0.97753 -0.00009 0.00214 0.01255 0.01469 -0.96284

D20 1.12861 -0.00020 0.00189 0.01141 0.01330 1.14191

D21 1.86839 -0.00016 0.00390 -0.01137 -0.00747 1.86092

D22 -1.10739 -0.00005 0.00527 -0.00457 0.00071 -1.10668

D23 2.49329 0.00018 0.00578 0.01930 0.02508 2.51837

D24 -0.81510 0.00004 0.00440 0.01234 0.01674 -0.79836

D25 -2.91283 -0.00029 -0.02427 -0.01029 -0.03456 -2.94739

D26 -0.79698 -0.00012 -0.02411 -0.01003 -0.03415 -0.83113

D27 1.23922 -0.00019 -0.02351 -0.01051 -0.03402 1.20519

D28 -3.09334 -0.00002 -0.00615 0.00510 -0.00104 -3.09439

D29 -0.97410 -0.00002 -0.00569 0.00476 -0.00093 -0.97504

D30 1.06621 -0.00004 -0.00622 0.00462 -0.00161 1.06461

D31 1.11208 0.00001 -0.00671 0.00564 -0.00107 1.11102

D32 -3.05187 0.00000 -0.00626 0.00531 -0.00095 -3.05282

D33 -1.01155 -0.00001 -0.00678 0.00516 -0.00163 -1.01318

D34 -0.98708 0.00002 -0.00709 0.00551 -0.00158 -0.98866

D35 1.13216 0.00001 -0.00664 0.00517 -0.00147 1.13069

D36 -3.11071 -0.00001 -0.00717 0.00502 -0.00215 -3.11285

D37 -3.10406 -0.00011 -0.00168 -0.00738 -0.00906 -3.11312

D38 -0.97387 -0.00006 -0.00201 -0.00635 -0.00836 -0.98224

D39 1.04743 -0.00007 -0.00178 -0.00675 -0.00853 1.03890

D40 1.05226 -0.00010 -0.00163 -0.00738 -0.00902 1.04324

D41 -3.10074 -0.00005 -0.00197 -0.00635 -0.00832 -3.10906

D42 -1.07943 -0.00006 -0.00173 -0.00675 -0.00849 -1.08792

D43 -0.97825 -0.00008 -0.00123 -0.00721 -0.00844 -0.98668

D44 1.15193 -0.00003 -0.00156 -0.00618 -0.00774 1.14420

D45 -3.10994 -0.00004 -0.00133 -0.00658 -0.00791 -3.11785

D46 -3.12206 0.00000 -0.00378 0.00103 -0.00275 -3.12480

D47 -1.02767 0.00000 -0.00375 0.00107 -0.00268 -1.03035

D48 1.06601 -0.00004 -0.00379 0.00086 -0.00293 1.06308

D49 1.03409 -0.00002 -0.00341 0.00001 -0.00339 1.03070

D50 3.12848 -0.00002 -0.00338 0.00005 -0.00333 3.12515

D51 -1.06103 -0.00005 -0.00342 -0.00016 -0.00358 -1.06461

D52 -0.99437 -0.00002 -0.00340 0.00037 -0.00304 -0.99741

D53 1.10002 -0.00002 -0.00338 0.00040 -0.00298 1.09705

D54 -3.08949 -0.00005 -0.00342 0.00020 -0.00322 -3.09271

Item Value Threshold Converged?

Maximum Force 0.000854 0.000450 NO

RMS Force 0.000178 0.000300 YES

Maximum Displacement 0.137545 0.001800 NO

RMS Displacement 0.034144 0.001200 NO

Predicted change in Energy=-1.636949D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:36:06 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.101030 -0.410450 -0.240609

2 6 0 -2.840176 0.046858 0.437472

3 8 0 -4.869731 0.315861 -0.829235

4 8 0 -4.288663 -1.746740 -0.169240

5 6 0 -2.392863 -0.778590 1.628865

6 16 0 -1.518636 0.080334 -0.928700

7 6 0 -0.098715 0.668324 -0.076069

8 16 0 1.123359 -0.605341 0.221042

9 16 0 -0.022090 2.235788 0.633860

10 6 0 2.709489 0.310275 0.037346

11 6 0 3.884723 -0.659566 -0.015631

12 6 0 5.226003 0.074832 -0.101534

13 6 0 6.415643 -0.878252 -0.195730

14 1 0 -2.986182 1.090144 0.713944

15 1 0 -5.102914 -1.951623 -0.659249

16 1 0 -1.481680 -0.350254 2.049502

17 1 0 -3.160006 -0.770208 2.410173

18 1 0 -2.192657 -1.814559 1.353649

19 1 0 2.642902 0.895996 -0.882091

20 1 0 2.810812 1.002673 0.873624

21 1 0 3.881088 -1.299878 0.874769

22 1 0 3.776204 -1.325209 -0.879472

23 1 0 5.218617 0.740646 -0.972809

24 1 0 5.340780 0.720942 0.776751

25 1 0 7.363285 -0.332686 -0.238982

26 1 0 6.460018 -1.546620 0.670542

27 1 0 6.354583 -1.504333 -1.091967

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.502890 0.000000

3 O 1.210334 2.407489 0.000000

4 O 1.351285 2.383948 2.242221 0.000000

5 C 2.558964 1.516862 3.657178 2.786495 0.000000

6 S 2.717185 1.901055 3.360834 3.404119 2.836046

7 C 4.148416 2.857543 4.842942 4.837033 3.203666

8 S 5.248366 4.022662 6.153765 5.544826 3.791543

9 S 4.940144 3.573736 5.415385 5.891447 3.961953

10 C 6.854187 5.570302 7.628602 7.297131 5.454590

11 C 7.992805 6.777064 8.846122 8.246805 6.490502

12 C 9.340685 8.084216 10.124796 9.687703 7.859373

13 C 10.527169 9.323463 11.366042 10.739514 8.996047

14 H 2.099009 1.089128 2.555127 3.244130 2.163624

15 H 1.885271 3.211963 2.285771 0.972158 3.735753

16 H 3.479832 2.145192 4.495523 3.840852 1.091175

17 H 2.835771 2.159036 3.820533 2.980076 1.094998

18 H 2.855708 2.173369 4.058374 2.591724 1.090440

19 H 6.899197 5.703194 7.535185 7.452436 5.870951

20 H 7.142268 5.747823 7.896973 7.684360 5.551713

21 H 8.108598 6.868793 9.060413 8.248301 6.340573

22 H 7.955862 6.884285 8.800445 8.107046 6.681911

23 H 9.418968 8.210625 10.098308 9.860080 8.186049

24 H 9.563622 8.215689 10.343976 9.985516 7.923631

25 H 11.464579 10.232900 12.264407 11.737645 9.943344

26 H 10.660995 9.438596 11.579352 10.783294 8.937660

27 H 10.547096 9.449283 11.373977 10.685920 9.189529

6 7 8 9 10

6 S 0.000000

7 C 1.757524 0.000000

8 S 2.961789 1.789961 0.000000

9 S 3.054050 1.722444 3.091032 0.000000

10 C 4.343174 2.833208 1.840626 3.394842 0.000000

11 C 5.529687 4.199371 2.772018 4.905924 1.524654

12 C 6.795174 5.357752 4.171137 5.723025 2.531317

13 C 8.025517 6.696497 5.315680 7.199297 3.899039

14 H 2.423156 3.023164 4.472801 3.178798 5.788493

15 H 4.128983 5.678577 6.430697 6.709792 8.163031

16 H 3.009395 2.732791 3.192893 3.289690 4.695846

17 H 3.816489 4.197889 4.813179 4.694445 6.422517

18 H 3.042045 3.548718 3.706882 4.651319 5.502601

19 H 4.240976 2.866700 2.404147 3.345942 1.092184

20 H 4.779456 3.078806 2.420551 3.098934 1.090432

21 H 5.857858 4.540566 2.918015 5.271979 2.160212

22 H 5.478440 4.431097 2.960900 5.421983 2.157137

23 H 6.769677 5.392901 4.473041 5.681711 2.738860

24 H 7.097220 5.506194 4.455837 5.574545 2.763885

25 H 8.918229 7.530604 6.262798 7.867825 4.706120

26 H 8.298402 6.962785 5.437645 7.505043 4.232666

27 H 8.032770 6.884587 5.467896 7.591372 4.225501

11 12 13 14 15

11 C 0.000000

12 C 1.531585 0.000000

13 C 2.546727 1.527248 0.000000

14 H 7.127629 8.314797 9.648648 0.000000

15 H 9.102817 10.540593 11.577744 3.952032 0.000000

16 H 5.758362 7.056960 8.227246 2.474265 4.797401

17 H 7.451508 8.794766 9.924488 2.523552 3.819946

18 H 6.335889 7.792553 8.796596 3.078344 3.541206

19 H 2.170862 2.820636 4.225237 5.854196 8.255680

20 H 2.169584 2.764954 4.204308 5.799853 8.585140

21 H 1.096734 2.156802 2.783471 7.273065 9.137301

22 H 1.095938 2.160376 2.762954 7.355458 8.903911

23 H 2.157789 1.096577 2.158137 8.383675 10.671487

24 H 2.157261 1.096365 2.158349 8.335380 10.875452

25 H 3.501018 2.180122 1.094320 10.490185 12.577905

26 H 2.808887 2.178991 1.095040 9.807401 11.646192

27 H 2.823533 2.179085 1.094964 9.861162 11.474387

16 17 18 19 20

16 H 0.000000

17 H 1.767264 0.000000

18 H 1.770280 1.772759 0.000000

19 H 5.211483 6.876698 5.977313 0.000000

20 H 4.651730 6.415197 5.762111 1.766949 0.000000

21 H 5.571451 7.225996 6.114295 3.072706 2.539140

22 H 6.097112 7.696804 6.391682 2.493618 3.069912

23 H 7.430909 9.161253 8.177314 2.581989 3.045570

24 H 7.022345 8.783790 7.969583 3.171900 2.547449

25 H 9.136240 10.860437 9.800431 4.919884 4.872995

26 H 8.148828 9.806834 8.683733 4.790346 4.456101

27 H 8.521018 10.165201 8.895650 4.425178 4.765180

21 22 23 24 25

21 H 0.000000

22 H 1.757556 0.000000

23 H 3.060436 2.521314 0.000000

24 H 2.494799 3.062305 1.753931 0.000000

25 H 3.781745 3.776570 2.508016 2.496471 0.000000

26 H 2.598744 3.107157 3.077867 2.530970 1.765435

27 H 3.166706 2.593314 2.518838 3.077621 1.765735

26 27

26 H 0.000000

27 H 1.766167 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 6.96D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.119697 -0.414209 -0.189787

2 6 0 -2.850592 0.119602 0.412789

3 8 0 -4.889464 0.233900 -0.862335

4 8 0 -4.313978 -1.728446 0.057213

5 6 0 -2.397557 -0.545887 1.698383

6 16 0 -1.540679 -0.034447 -0.956300

7 6 0 -0.110305 0.650707 -0.199013

8 16 0 1.107329 -0.581116 0.252584

9 16 0 -0.019055 2.297003 0.299178

10 6 0 2.696780 0.292264 -0.061671

11 6 0 3.866221 -0.683816 0.003484

12 6 0 5.210690 0.024288 -0.188207

13 6 0 6.394273 -0.940664 -0.166220

14 1 0 -2.988540 1.191009 0.551561

15 1 0 -5.133512 -1.990325 -0.395416

16 1 0 -1.480476 -0.072180 2.052256

17 1 0 -3.157900 -0.430424 2.477849

18 1 0 -2.205363 -1.610230 1.559478

19 1 0 2.625483 0.753166 -1.049271

20 1 0 2.809051 1.087384 0.676043

21 1 0 3.866754 -1.202178 0.969986

22 1 0 3.746663 -1.455969 -0.764999

23 1 0 5.199439 0.570504 -1.138998

24 1 0 5.336523 0.778922 0.597102

25 1 0 7.344462 -0.411625 -0.287855

26 1 0 6.442453 -1.490307 0.779658

27 1 0 6.322108 -1.678139 -0.972364

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3303347 0.1915352 0.1798144

Leave Link 202 at Sat Aug 17 17:36:06 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1101.0401264716 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0548624099 Hartrees.

Nuclear repulsion after empirical dispersion term = 1100.9852640618 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2319

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.43D-09

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 93

GePol: Fraction of low-weight points (<1% of avg) = 4.01%

GePol: Cavity surface area = 309.178 Ang\*\*2

GePol: Cavity volume = 319.949 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0058178687 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1100.9794461931 Hartrees.

Leave Link 301 at Sat Aug 17 17:36:06 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.86D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:36:06 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:36:06 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999987 -0.005021 -0.000668 -0.000144 Ang= -0.58 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.62957219036

Leave Link 401 at Sat Aug 17 17:36:07 2019, MaxMem= 1342177280 cpu: 7.5

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16133283.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.88D-15 for 2304.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.53D-15 for 683 468.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.88D-15 for 2307.

Iteration 1 A^-1\*A deviation from orthogonality is 1.77D-09 for 649 562.

Iteration 2 A\*A^-1 deviation from unit magnitude is 3.11D-15 for 394.

Iteration 2 A\*A^-1 deviation from orthogonality is 4.11D-15 for 2287 48.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 485.

Iteration 2 A^-1\*A deviation from orthogonality is 7.50D-16 for 2287 2185.

E= -1658.67482780557

DIIS: error= 1.75D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67482780557 IErMin= 1 ErrMin= 1.75D-03

ErrMax= 1.75D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.50D-03 BMatP= 4.50D-03

IDIUse=3 WtCom= 9.83D-01 WtEn= 1.75D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.428 Goal= None Shift= 0.000

Gap= 0.483 Goal= None Shift= 0.000

GapD= 0.428 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=1.65D-04 MaxDP=5.41D-03 OVMax= 8.91D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.65D-04 CP: 1.00D+00

E= -1658.67687734306 Delta-E= -0.002049537488 Rises=F Damp=F

DIIS: error= 2.21D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67687734306 IErMin= 2 ErrMin= 2.21D-04

ErrMax= 2.21D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.43D-05 BMatP= 4.50D-03

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.21D-03

Coeff-Com: -0.641D-01 0.106D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.639D-01 0.106D+01

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.76D-05 MaxDP=8.82D-04 DE=-2.05D-03 OVMax= 1.78D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.67D-05 CP: 1.00D+00 1.04D+00

E= -1658.67689528368 Delta-E= -0.000017940625 Rises=F Damp=F

DIIS: error= 1.82D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67689528368 IErMin= 3 ErrMin= 1.82D-04

ErrMax= 1.82D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.26D-05 BMatP= 8.43D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.82D-03

Coeff-Com: -0.362D-01 0.496D+00 0.541D+00

Coeff-En: 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.361D-01 0.495D+00 0.541D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.86D-05 MaxDP=8.85D-04 DE=-1.79D-05 OVMax= 1.95D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.32D-05 CP: 1.00D+00 1.08D+00 5.57D-01

E= -1658.67690344904 Delta-E= -0.000008165356 Rises=F Damp=F

DIIS: error= 1.16D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67690344904 IErMin= 4 ErrMin= 1.16D-04

ErrMax= 1.16D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.98D-05 BMatP= 5.26D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.16D-03

Coeff-Com: -0.132D-01 0.169D+00 0.377D+00 0.468D+00

Coeff-En: 0.000D+00 0.000D+00 0.289D+00 0.711D+00

Coeff: -0.132D-01 0.169D+00 0.377D+00 0.468D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=7.35D-06 MaxDP=3.28D-04 DE=-8.17D-06 OVMax= 6.93D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.21D-06 CP: 1.00D+00 1.08D+00 6.60D-01 6.04D-01

E= -1658.67690795838 Delta-E= -0.000004509338 Rises=F Damp=F

DIIS: error= 2.17D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67690795838 IErMin= 5 ErrMin= 2.17D-05

ErrMax= 2.17D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.21D-07 BMatP= 1.98D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.250D-02 0.256D-01 0.117D+00 0.192D+00 0.668D+00

Coeff: -0.250D-02 0.256D-01 0.117D+00 0.192D+00 0.668D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.52D-06 MaxDP=5.53D-05 DE=-4.51D-06 OVMax= 1.33D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.13D-06 CP: 1.00D+00 1.08D+00 6.83D-01 6.64D-01 9.44D-01

E= -1658.67690804310 Delta-E= -0.000000084722 Rises=F Damp=F

DIIS: error= 1.53D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67690804310 IErMin= 6 ErrMin= 1.53D-05

ErrMax= 1.53D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.70D-07 BMatP= 4.21D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.102D-02-0.184D-01 0.413D-02 0.350D-01 0.427D+00 0.551D+00

Coeff: 0.102D-02-0.184D-01 0.413D-02 0.350D-01 0.427D+00 0.551D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=7.38D-07 MaxDP=2.66D-05 DE=-8.47D-08 OVMax= 8.16D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.18D-07 CP: 1.00D+00 1.08D+00 6.92D-01 6.88D-01 1.01D+00

CP: 8.24D-01

E= -1658.67690808077 Delta-E= -0.000000037674 Rises=F Damp=F

DIIS: error= 3.29D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67690808077 IErMin= 7 ErrMin= 3.29D-06

ErrMax= 3.29D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.12D-09 BMatP= 1.70D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.643D-03-0.967D-02-0.103D-01-0.754D-02 0.884D-01 0.208D+00

Coeff-Com: 0.731D+00

Coeff: 0.643D-03-0.967D-02-0.103D-01-0.754D-02 0.884D-01 0.208D+00

Coeff: 0.731D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.35D-07 MaxDP=1.28D-05 DE=-3.77D-08 OVMax= 4.54D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.02D-07 CP: 1.00D+00 1.08D+00 6.94D-01 6.92D-01 1.06D+00

CP: 9.17D-01 1.16D+00

E= -1658.67690808334 Delta-E= -0.000000002563 Rises=F Damp=F

DIIS: error= 2.23D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67690808334 IErMin= 8 ErrMin= 2.23D-06

ErrMax= 2.23D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.11D-09 BMatP= 8.12D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.187D-03-0.211D-02-0.723D-02-0.123D-01-0.332D-01 0.162D-01

Coeff-Com: 0.462D+00 0.577D+00

Coeff: 0.187D-03-0.211D-02-0.723D-02-0.123D-01-0.332D-01 0.162D-01

Coeff: 0.462D+00 0.577D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.78D-07 MaxDP=6.07D-06 DE=-2.56D-09 OVMax= 2.25D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 9.52D-08 CP: 1.00D+00 1.08D+00 6.95D-01 6.98D-01 1.07D+00

CP: 9.84D-01 1.32D+00 7.94D-01

E= -1658.67690808450 Delta-E= -0.000000001166 Rises=F Damp=F

DIIS: error= 6.75D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67690808450 IErMin= 9 ErrMin= 6.75D-07

ErrMax= 6.75D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.42D-10 BMatP= 4.11D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.493D-04 0.124D-02-0.188D-02-0.590D-02-0.427D-01-0.412D-01

Coeff-Com: 0.965D-01 0.348D+00 0.646D+00

Coeff: -0.493D-04 0.124D-02-0.188D-02-0.590D-02-0.427D-01-0.412D-01

Coeff: 0.965D-01 0.348D+00 0.646D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=8.15D-08 MaxDP=3.12D-06 DE=-1.17D-09 OVMax= 1.24D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 3.26D-08 CP: 1.00D+00 1.08D+00 6.96D-01 6.99D-01 1.07D+00

CP: 1.01D+00 1.40D+00 9.37D-01 8.14D-01

E= -1658.67690808472 Delta-E= -0.000000000216 Rises=F Damp=F

DIIS: error= 1.92D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67690808472 IErMin=10 ErrMin= 1.92D-07

ErrMax= 1.92D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.78D-11 BMatP= 7.42D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.518D-04 0.976D-03-0.715D-04-0.159D-02-0.183D-01-0.241D-01

Coeff-Com: -0.100D-01 0.113D+00 0.341D+00 0.599D+00

Coeff: -0.518D-04 0.976D-03-0.715D-04-0.159D-02-0.183D-01-0.241D-01

Coeff: -0.100D-01 0.113D+00 0.341D+00 0.599D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.38D-08 MaxDP=1.01D-06 DE=-2.16D-10 OVMax= 3.23D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.17D-08 CP: 1.00D+00 1.08D+00 6.96D-01 7.00D-01 1.08D+00

CP: 1.01D+00 1.43D+00 9.72D-01 9.06D-01 8.32D-01

E= -1658.67690808474 Delta-E= -0.000000000027 Rises=F Damp=F

DIIS: error= 3.18D-08 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67690808474 IErMin=11 ErrMin= 3.18D-08

ErrMax= 3.18D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.93D-12 BMatP= 8.78D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.654D-05 0.796D-04 0.181D-03 0.280D-03 0.946D-03-0.723D-03

Coeff-Com: -0.152D-01-0.143D-01-0.156D-02 0.154D+00 0.876D+00

Coeff: -0.654D-05 0.796D-04 0.181D-03 0.280D-03 0.946D-03-0.723D-03

Coeff: -0.152D-01-0.143D-01-0.156D-02 0.154D+00 0.876D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=9.53D-09 MaxDP=4.66D-07 DE=-2.68D-11 OVMax= 1.25D-06

Error on total polarization charges = 0.04175

SCF Done: E(UB3LYP) = -1658.67690808 A.U. after 11 cycles

NFock= 11 Conv=0.95D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655232944241D+03 PE=-6.144721403938D+03 EE= 1.729832105419D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.65

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:36:31 2019, MaxMem= 1342177280 cpu: 276.3

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 342

Leave Link 701 at Sat Aug 17 17:36:32 2019, MaxMem= 1342177280 cpu: 10.2

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:36:32 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:36:35 2019, MaxMem= 1342177280 cpu: 36.0

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.32693159D+00-2.88827180D+00 5.87905132D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000949187 -0.000402219 0.000623041

2 6 -0.000897593 -0.000102450 -0.000180592

3 8 -0.000482270 0.000287280 -0.000377065

4 8 -0.000051169 0.000194579 -0.000003005

5 6 0.000092406 -0.000151370 0.000178789

6 16 0.000326792 -0.000089839 -0.000013972

7 6 -0.000068873 0.000481352 0.000111885

8 16 0.000249881 -0.000081509 -0.000216155

9 16 -0.000079617 -0.000101897 0.000011984

10 6 -0.000103578 -0.000075649 0.000006153

11 6 -0.000089847 -0.000049248 0.000075730

12 6 0.000039528 0.000065049 -0.000004568

13 6 0.000111246 -0.000005509 -0.000040938

14 1 0.000204702 -0.000003118 0.000013038

15 1 -0.000006982 0.000075581 0.000013797

16 1 -0.000063935 0.000001348 -0.000058786

17 1 0.000024483 -0.000044943 -0.000061600

18 1 0.000045644 0.000081590 -0.000082146

19 1 0.000012229 0.000007354 0.000077056

20 1 -0.000057690 -0.000030468 -0.000064075

21 1 -0.000001721 -0.000002207 -0.000034177

22 1 -0.000004842 0.000045976 0.000011831

23 1 0.000012616 -0.000061603 0.000009809

24 1 -0.000008542 -0.000034538 -0.000000631

25 1 -0.000080227 0.000012206 -0.000047648

26 1 -0.000033096 0.000035340 -0.000025768

27 1 -0.000038732 -0.000051089 0.000078012

-------------------------------------------------------------------

Cartesian Forces: Max 0.000949187 RMS 0.000208848

Leave Link 716 at Sat Aug 17 17:36:35 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000658575 RMS 0.000130661

Search for a local minimum.

Step number 16 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .13066D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16

DE= -3.07D-05 DEPred=-1.64D-05 R= 1.88D+00

TightC=F SS= 1.41D+00 RLast= 7.96D-02 DXNew= 1.0000D-01 2.3886D-01

Trust test= 1.88D+00 RLast= 7.96D-02 DXMaxT set to 1.00D-01

ITU= 1 -1 1 -1 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Eigenvalues --- 0.00117 0.00235 0.00295 0.00377 0.00465

Eigenvalues --- 0.00511 0.00611 0.00940 0.01582 0.02302

Eigenvalues --- 0.02376 0.03235 0.03559 0.03719 0.04630

Eigenvalues --- 0.04786 0.04835 0.04956 0.05060 0.05448

Eigenvalues --- 0.05464 0.05582 0.05687 0.05821 0.08210

Eigenvalues --- 0.08282 0.08382 0.11307 0.12162 0.12220

Eigenvalues --- 0.13883 0.15395 0.15925 0.16001 0.16027

Eigenvalues --- 0.16048 0.16148 0.16408 0.17650 0.18491

Eigenvalues --- 0.19985 0.21913 0.21978 0.23031 0.23543

Eigenvalues --- 0.24051 0.24883 0.25379 0.25689 0.26470

Eigenvalues --- 0.27148 0.29116 0.29469 0.29612 0.29753

Eigenvalues --- 0.30288 0.31397 0.32680 0.33591 0.33871

Eigenvalues --- 0.33879 0.33894 0.33957 0.34027 0.34035

Eigenvalues --- 0.34099 0.34179 0.34442 0.34533 0.34547

Eigenvalues --- 0.34643 0.39172 0.52638 0.57137 1.39907

En-DIIS/RFO-DIIS IScMMF= 0 using points: 16 15 14 13 12

RFO step: Lambda=-6.79429299D-06.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= -6.45D-06 SmlDif= 1.00D-05

RMS Error= 0.7875656366D-03 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.58021 -1.00347 0.15857 1.07823 -0.81354

Iteration 1 RMS(Cart)= 0.05436875 RMS(Int)= 0.00085989

Iteration 2 RMS(Cart)= 0.00252236 RMS(Int)= 0.00000873

Iteration 3 RMS(Cart)= 0.00000294 RMS(Int)= 0.00000869

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000869

ITry= 1 IFail=0 DXMaxC= 2.05D-01 DCOld= 1.00D+10 DXMaxT= 1.00D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.84005 -0.00050 -0.00121 -0.00139 -0.00260 2.83745

R2 2.28720 0.00066 0.00042 -0.00184 -0.00142 2.28578

R3 2.55356 -0.00024 -0.00039 -0.00056 -0.00095 2.55261

R4 2.86645 0.00006 0.00053 -0.00063 -0.00010 2.86635

R5 3.59247 0.00018 0.00053 0.00115 0.00168 3.59415

R6 2.05815 -0.00003 -0.00011 -0.00091 -0.00102 2.05714

R7 1.83711 -0.00002 -0.00009 -0.00080 -0.00089 1.83622

R8 2.06202 -0.00007 -0.00011 -0.00103 -0.00114 2.06088

R9 2.06925 -0.00006 -0.00006 -0.00075 -0.00081 2.06843

R10 2.06063 -0.00006 -0.00010 -0.00070 -0.00080 2.05983

R11 3.32124 -0.00009 0.00033 -0.00002 0.00032 3.32156

R12 3.38254 0.00014 0.00101 0.00041 0.00142 3.38396

R13 3.25495 -0.00010 -0.00044 -0.00073 -0.00118 3.25377

R14 3.47828 -0.00028 -0.00135 -0.00141 -0.00276 3.47552

R15 2.88118 -0.00005 0.00003 -0.00060 -0.00057 2.88061

R16 2.06393 -0.00006 0.00005 -0.00087 -0.00082 2.06311

R17 2.06062 -0.00008 -0.00013 -0.00083 -0.00096 2.05966

R18 2.89428 -0.00001 -0.00016 -0.00030 -0.00046 2.89381

R19 2.07253 -0.00002 -0.00012 -0.00044 -0.00056 2.07197

R20 2.07102 -0.00004 -0.00003 -0.00057 -0.00060 2.07042

R21 2.88608 -0.00003 0.00012 -0.00063 -0.00051 2.88557

R22 2.07223 -0.00004 -0.00012 -0.00059 -0.00072 2.07151

R23 2.07183 -0.00002 -0.00007 -0.00045 -0.00051 2.07132

R24 2.06797 -0.00006 -0.00014 -0.00058 -0.00072 2.06725

R25 2.06933 -0.00004 -0.00012 -0.00050 -0.00062 2.06871

R26 2.06918 -0.00004 -0.00009 -0.00054 -0.00063 2.06855

A1 2.17689 0.00014 0.00116 0.00021 0.00136 2.17825

A2 1.97531 0.00006 -0.00066 -0.00051 -0.00118 1.97413

A3 2.13049 -0.00019 -0.00023 -0.00013 -0.00037 2.13012

A4 2.02216 -0.00006 -0.00148 0.00072 -0.00076 2.02140

A5 1.83830 0.00019 0.00126 0.00112 0.00238 1.84068

A6 1.86873 0.00006 0.00083 0.00219 0.00302 1.87175

A7 1.94876 -0.00019 0.00015 -0.00319 -0.00304 1.94572

A8 1.94060 0.00004 0.00059 -0.00106 -0.00047 1.94013

A9 1.83252 -0.00004 -0.00131 0.00044 -0.00087 1.83165

A10 1.87349 -0.00011 -0.00053 0.00113 0.00061 1.87410

A11 1.91284 -0.00007 0.00068 -0.00195 -0.00128 1.91156

A12 1.92801 0.00004 -0.00031 0.00134 0.00103 1.92904

A13 1.95294 -0.00010 -0.00086 0.00030 -0.00056 1.95238

A14 1.88280 0.00004 0.00002 0.00045 0.00046 1.88326

A15 1.89327 0.00005 0.00023 -0.00012 0.00011 1.89338

A16 1.89229 0.00005 0.00027 -0.00001 0.00027 1.89256

A17 1.79147 -0.00009 0.00033 0.00045 0.00077 1.79224

A18 1.97584 -0.00049 -0.00205 -0.00366 -0.00576 1.97008

A19 2.14165 0.00015 0.00083 0.00034 0.00112 2.14277

A20 2.15166 0.00030 0.00155 0.00072 0.00221 2.15388

A21 1.79036 0.00043 0.00143 0.00252 0.00395 1.79431

A22 1.92973 -0.00032 -0.00193 -0.00111 -0.00304 1.92669

A23 1.87366 0.00007 0.00139 -0.00093 0.00046 1.87412

A24 1.89589 0.00011 -0.00027 0.00079 0.00052 1.89641

A25 1.93786 0.00016 0.00053 0.00083 0.00136 1.93922

A26 1.93792 0.00005 0.00012 0.00057 0.00069 1.93861

A27 1.88679 -0.00006 0.00024 -0.00019 0.00005 1.88684

A28 1.95194 0.00013 0.00087 0.00080 0.00167 1.95360

A29 1.91837 -0.00007 -0.00067 0.00024 -0.00043 1.91794

A30 1.91497 -0.00001 0.00011 -0.00053 -0.00042 1.91455

A31 1.90539 0.00001 0.00032 0.00033 0.00066 1.90605

A32 1.91107 -0.00008 -0.00065 -0.00026 -0.00091 1.91016

A33 1.85980 0.00002 -0.00004 -0.00064 -0.00068 1.85912

A34 1.96750 -0.00005 -0.00058 -0.00017 -0.00075 1.96675

A35 1.90689 -0.00003 -0.00002 -0.00045 -0.00047 1.90642

A36 1.90639 0.00005 0.00035 0.00088 0.00123 1.90762

A37 1.91256 0.00003 0.00003 0.00007 0.00010 1.91266

A38 1.91307 -0.00002 -0.00003 -0.00015 -0.00017 1.91290

A39 1.85395 0.00001 0.00030 -0.00018 0.00012 1.85407

A40 1.94535 -0.00005 -0.00008 0.00029 0.00021 1.94556

A41 1.94300 -0.00006 -0.00021 -0.00023 -0.00044 1.94256

A42 1.94321 0.00004 -0.00023 0.00085 0.00062 1.94383

A43 1.87598 0.00006 0.00031 -0.00017 0.00014 1.87612

A44 1.87654 0.00003 0.00026 -0.00003 0.00023 1.87677

A45 1.87631 -0.00002 -0.00001 -0.00078 -0.00079 1.87551

D1 2.63686 0.00009 -0.01442 0.01936 0.00494 2.64180

D2 -1.48347 -0.00004 -0.01424 0.01658 0.00234 -1.48112

D3 0.46076 0.00002 -0.01482 0.01848 0.00367 0.46443

D4 -0.53805 0.00013 -0.00607 0.00487 -0.00120 -0.53925

D5 1.62481 0.00000 -0.00588 0.00209 -0.00379 1.62102

D6 -2.71415 0.00006 -0.00647 0.00400 -0.00247 -2.71661

D7 -3.10483 -0.00005 -0.00566 0.00749 0.00182 -3.10300

D8 0.00445 0.00000 0.00248 -0.00656 -0.00408 0.00037

D9 -3.12694 0.00000 0.00163 0.00770 0.00933 -3.11761

D10 -1.05472 0.00003 0.00188 0.00785 0.00973 -1.04499

D11 1.05532 0.00005 0.00144 0.00897 0.01041 1.06573

D12 1.05199 -0.00007 0.00094 0.00819 0.00913 1.06112

D13 3.12421 -0.00004 0.00119 0.00835 0.00953 3.13374

D14 -1.04893 -0.00002 0.00074 0.00947 0.01021 -1.03872

D15 -0.98837 0.00008 0.00210 0.01034 0.01244 -0.97592

D16 1.08385 0.00010 0.00235 0.01050 0.01285 1.09670

D17 -3.08929 0.00012 0.00190 0.01162 0.01352 -3.07577

D18 3.11173 0.00005 0.00134 0.02757 0.02891 3.14064

D19 -0.96284 0.00000 0.00046 0.02723 0.02769 -0.93515

D20 1.14191 -0.00008 0.00044 0.02449 0.02494 1.16685

D21 1.86092 -0.00020 0.00255 -0.01619 -0.01363 1.84728

D22 -1.10668 0.00002 0.00078 -0.00032 0.00046 -1.10623

D23 2.51837 0.00006 -0.00055 0.03091 0.03036 2.54873

D24 -0.79836 -0.00019 0.00115 0.01488 0.01603 -0.78233

D25 -2.94739 -0.00018 -0.03590 -0.03080 -0.06670 -3.01409

D26 -0.83113 -0.00014 -0.03553 -0.03102 -0.06655 -0.89768

D27 1.20519 -0.00011 -0.03464 -0.03133 -0.06597 1.13922

D28 -3.09439 -0.00005 -0.00735 -0.00449 -0.01184 -3.10623

D29 -0.97504 0.00000 -0.00682 -0.00337 -0.01019 -0.98523

D30 1.06461 -0.00003 -0.00719 -0.00432 -0.01152 1.05309

D31 1.11102 -0.00003 -0.00817 -0.00315 -0.01132 1.09970

D32 -3.05282 0.00001 -0.00764 -0.00203 -0.00967 -3.06249

D33 -1.01318 -0.00001 -0.00801 -0.00298 -0.01099 -1.02417

D34 -0.98866 -0.00009 -0.00891 -0.00386 -0.01276 -1.00142

D35 1.13069 -0.00004 -0.00837 -0.00274 -0.01111 1.11958

D36 -3.11285 -0.00007 -0.00875 -0.00369 -0.01244 -3.12529

D37 -3.11312 -0.00004 -0.00472 -0.00670 -0.01142 -3.12454

D38 -0.98224 -0.00005 -0.00509 -0.00705 -0.01214 -0.99438

D39 1.03890 -0.00002 -0.00455 -0.00703 -0.01158 1.02733

D40 1.04324 -0.00004 -0.00468 -0.00775 -0.01243 1.03081

D41 -3.10906 -0.00005 -0.00505 -0.00810 -0.01315 -3.12221

D42 -1.08792 -0.00002 -0.00450 -0.00808 -0.01258 -1.10051

D43 -0.98668 -0.00002 -0.00445 -0.00703 -0.01147 -0.99816

D44 1.14420 -0.00004 -0.00482 -0.00737 -0.01219 1.13201

D45 -3.11785 -0.00001 -0.00427 -0.00735 -0.01163 -3.12947

D46 -3.12480 -0.00005 -0.00435 -0.01171 -0.01606 -3.14087

D47 -1.03035 -0.00005 -0.00415 -0.01189 -0.01604 -1.04639

D48 1.06308 -0.00008 -0.00446 -0.01246 -0.01692 1.04615

D49 1.03070 0.00000 -0.00395 -0.01107 -0.01502 1.01568

D50 3.12515 0.00000 -0.00375 -0.01125 -0.01500 3.11016

D51 -1.06461 -0.00003 -0.00406 -0.01182 -0.01588 -1.08049

D52 -0.99741 -0.00002 -0.00431 -0.01081 -0.01512 -1.01253

D53 1.09705 -0.00002 -0.00411 -0.01099 -0.01510 1.08195

D54 -3.09271 -0.00006 -0.00442 -0.01156 -0.01598 -3.10869

Item Value Threshold Converged?

Maximum Force 0.000659 0.000450 NO

RMS Force 0.000131 0.000300 YES

Maximum Displacement 0.204898 0.001800 NO

RMS Displacement 0.054961 0.001200 NO

Predicted change in Energy=-3.376779D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:36:35 2019, MaxMem= 1342177280 cpu: 0.6

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.107431 -0.412034 -0.202168

2 6 0 -2.839623 0.056338 0.451926

3 8 0 -4.907761 0.309123 -0.752164

4 8 0 -4.259388 -1.753696 -0.163942

5 6 0 -2.339571 -0.791347 1.606086

6 16 0 -1.554524 0.156537 -0.946599

7 6 0 -0.112371 0.708416 -0.106893

8 16 0 1.104105 -0.587215 0.112614

9 16 0 -0.016803 2.240552 0.672912

10 6 0 2.697036 0.322354 -0.020742

11 6 0 3.866868 -0.654824 -0.037089

12 6 0 5.215387 0.068279 -0.097295

13 6 0 6.399106 -0.895454 -0.138437

14 1 0 -2.998352 1.087755 0.761782

15 1 0 -5.081051 -1.966302 -0.637058

16 1 0 -1.432633 -0.347479 2.018147

17 1 0 -3.087127 -0.831878 2.404581

18 1 0 -2.113947 -1.810779 1.293053

19 1 0 2.661665 0.908761 -0.940957

20 1 0 2.775284 1.013358 0.818500

21 1 0 3.836629 -1.287885 0.857614

22 1 0 3.774644 -1.326845 -0.897477

23 1 0 5.238346 0.716480 -0.981014

24 1 0 5.310400 0.730522 0.770938

25 1 0 7.351315 -0.358571 -0.180400

26 1 0 6.421368 -1.536076 0.748977

27 1 0 6.350589 -1.549727 -1.014671

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.501515 0.000000

3 O 1.209583 2.406435 0.000000

4 O 1.350782 2.381438 2.240896 0.000000

5 C 2.557145 1.516809 3.656225 2.782950 0.000000

6 S 2.719335 1.901944 3.362334 3.402621 2.833899

7 C 4.150299 2.859263 4.855057 4.823173 3.184966

8 S 5.223971 4.010272 6.139527 5.495836 3.759126

9 S 4.953303 3.576023 5.448187 5.886754 3.931727

10 C 6.846386 5.563161 7.639901 7.261013 5.408725

11 C 7.979702 6.761798 8.856334 8.201198 6.421725

12 C 9.335771 8.073721 10.147167 9.648595 7.792166

13 C 10.517845 9.306372 11.387402 10.693022 8.911716

14 H 2.099672 1.088590 2.558153 3.243612 2.162838

15 H 1.884891 3.209510 2.284915 0.971685 3.732014

16 H 3.476853 2.143767 4.492468 3.837903 1.090573

17 H 2.830624 2.159410 3.818590 2.970059 1.094567

18 H 2.857648 2.172608 4.059839 2.594033 1.090017

19 H 6.936207 5.738547 7.595488 7.456099 5.864313

20 H 7.102483 5.707665 7.873508 7.622886 5.480784

21 H 8.062155 6.822306 9.033614 8.173497 6.241171

22 H 7.965390 6.890762 8.836383 8.078734 6.628590

23 H 9.445829 8.230595 10.156860 9.847656 8.148095

24 H 9.536661 8.184080 10.339644 9.931071 7.844464

25 H 11.458891 10.218963 12.290552 11.694232 9.863675

26 H 10.631262 9.401594 11.576154 10.721908 8.834212

27 H 10.551051 9.444064 11.413794 10.645983 9.108369

6 7 8 9 10

6 S 0.000000

7 C 1.757692 0.000000

8 S 2.956925 1.790714 0.000000

9 S 3.054590 1.721822 3.092997 0.000000

10 C 4.354361 2.837117 1.839165 3.394932 0.000000

11 C 5.556708 4.206857 2.767643 4.895938 1.524353

12 C 6.823547 5.366086 4.168498 5.717325 2.532293

13 C 8.063501 6.706171 5.309904 7.187260 3.899004

14 H 2.422885 3.037661 4.478515 3.197886 5.799623

15 H 4.127790 5.667713 6.381225 6.712693 8.131200

16 H 3.009752 2.715474 3.181755 3.242242 4.654020

17 H 3.815265 4.186787 4.783241 4.676045 6.377381

18 H 3.033039 3.508917 3.639560 4.603897 5.424192

19 H 4.282771 2.903632 2.402905 3.398887 1.091751

20 H 4.753625 3.047605 2.419287 3.053351 1.089925

21 H 5.865669 4.528807 2.917645 5.228090 2.159410

22 H 5.531986 4.458273 2.949427 5.437602 2.156330

23 H 6.815996 5.421654 4.470749 5.716193 2.745126

24 H 7.099758 5.493407 4.456763 5.537950 2.760984

25 H 8.953567 7.539925 6.258256 7.859564 4.706534

26 H 8.327951 6.961322 5.438620 7.464499 4.232833

27 H 8.087446 6.906021 5.451862 7.599857 4.223865

11 12 13 14 15

11 C 0.000000

12 C 1.531341 0.000000

13 C 2.545664 1.526979 0.000000

14 H 7.127835 8.321229 9.646540 0.000000

15 H 9.063399 10.509400 11.540769 3.952424 0.000000

16 H 5.692378 6.988856 8.141699 2.467757 4.793919

17 H 7.372324 8.717879 9.821385 2.528174 3.809753

18 H 6.235035 7.693053 8.680960 3.076674 3.543052

19 H 2.171241 2.817742 4.227020 5.913304 8.264865

20 H 2.169429 2.772356 4.206112 5.774394 8.527545

21 H 1.096437 2.156850 2.777122 7.236700 9.067487

22 H 1.095621 2.159260 2.765871 7.379493 8.882570

23 H 2.156947 1.096198 2.157691 8.427241 10.667970

24 H 2.157747 1.096094 2.157786 8.316433 10.827629

25 H 3.499953 2.179747 1.093940 10.492625 12.544204

26 H 2.814245 2.178192 1.094713 9.778332 11.593611

27 H 2.815206 2.179038 1.094630 9.874958 11.445458

16 17 18 19 20

16 H 0.000000

17 H 1.766728 0.000000

18 H 1.769519 1.772236 0.000000

19 H 5.205546 6.875396 5.932383 0.000000

20 H 4.582313 6.347316 5.666174 1.766222 0.000000

21 H 5.476890 7.109111 5.989356 3.072564 2.534503

22 H 6.047789 7.631021 6.301438 2.497708 3.069177

23 H 7.391139 9.119933 8.100286 2.584156 3.064810

24 H 6.941621 8.696456 7.864587 3.158821 2.551288

25 H 9.054914 10.764164 9.688713 4.917051 4.880579

26 H 8.044183 9.677210 8.557048 4.792543 4.449537

27 H 8.439308 10.063652 8.777363 4.433706 4.765787

21 22 23 24 25

21 H 0.000000

22 H 1.756617 0.000000

23 H 3.059876 2.514872 0.000000

24 H 2.500695 3.061848 1.753489 0.000000

25 H 3.780755 3.774166 2.502270 2.501300 0.000000

26 H 2.598898 3.124058 3.076755 2.524322 1.764954

27 H 3.145474 2.588224 2.524660 3.077325 1.765308

26 27

26 H 0.000000

27 H 1.765121 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 7.36D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.117377 -0.430748 -0.147265

2 6 0 -2.843358 0.116019 0.429334

3 8 0 -4.918843 0.213005 -0.784702

4 8 0 -4.273995 -1.754187 0.073170

5 6 0 -2.338443 -0.569966 1.684402

6 16 0 -1.567615 0.020162 -0.978033

7 6 0 -0.117664 0.673987 -0.229946

8 16 0 1.095534 -0.585578 0.155157

9 16 0 -0.011068 2.297101 0.334686

10 6 0 2.690835 0.290276 -0.110217

11 6 0 3.856928 -0.685471 -0.001599

12 6 0 5.207645 0.016652 -0.167703

13 6 0 6.387502 -0.949192 -0.085559

14 1 0 -2.996146 1.180596 0.597742

15 1 0 -5.099691 -2.025096 -0.361578

16 1 0 -1.427048 -0.078576 2.026812

17 1 0 -3.080595 -0.498647 2.485776

18 1 0 -2.118740 -1.623403 1.510799

19 1 0 2.651247 0.746920 -1.101090

20 1 0 2.777432 1.088127 0.627260

21 1 0 3.830560 -1.191491 0.970730

22 1 0 3.756278 -1.467310 -0.762507

23 1 0 5.226865 0.539193 -1.131151

24 1 0 5.311101 0.789853 0.602284

25 1 0 7.341363 -0.427291 -0.205862

26 1 0 6.413554 -1.463931 0.880237

27 1 0 6.330513 -1.715791 -0.864848

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3279524 0.1922489 0.1801316

Leave Link 202 at Sat Aug 17 17:36:35 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1101.9135512069 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0549634194 Hartrees.

Nuclear repulsion after empirical dispersion term = 1101.8585877875 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

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Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2314

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.46D-10

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 95

GePol: Fraction of low-weight points (<1% of avg) = 4.11%

GePol: Cavity surface area = 309.389 Ang\*\*2

GePol: Cavity volume = 320.128 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057571912 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1101.8528305962 Hartrees.

Leave Link 301 at Sat Aug 17 17:36:35 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:36:35 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:36:35 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999987 -0.005020 -0.001033 -0.000374 Ang= -0.59 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.63008349503

Leave Link 401 at Sat Aug 17 17:36:36 2019, MaxMem= 1342177280 cpu: 7.5

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16063788.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.00D-15 for 2313.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.24D-15 for 703 444.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.00D-15 for 2313.

Iteration 1 A^-1\*A deviation from orthogonality is 1.78D-09 for 747 707.

Iteration 2 A\*A^-1 deviation from unit magnitude is 7.99D-15 for 577.

Iteration 2 A\*A^-1 deviation from orthogonality is 4.36D-15 for 1156 536.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.55D-15 for 568.

Iteration 2 A^-1\*A deviation from orthogonality is 4.18D-16 for 2046 1928.

E= -1658.67164291730

DIIS: error= 2.93D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67164291730 IErMin= 1 ErrMin= 2.93D-03

ErrMax= 2.93D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.13D-02 BMatP= 1.13D-02

IDIUse=3 WtCom= 9.71D-01 WtEn= 2.93D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.428 Goal= None Shift= 0.000

Gap= 0.484 Goal= None Shift= 0.000

GapD= 0.428 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=2.61D-04 MaxDP=7.97D-03 OVMax= 1.46D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.61D-04 CP: 1.00D+00

E= -1658.67686222234 Delta-E= -0.005219305044 Rises=F Damp=F

DIIS: error= 2.50D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67686222234 IErMin= 2 ErrMin= 2.50D-04

ErrMax= 2.50D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.97D-04 BMatP= 1.13D-02

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.50D-03

Coeff-Com: -0.628D-01 0.106D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.626D-01 0.106D+01

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.34D-05 MaxDP=1.42D-03 DE=-5.22D-03 OVMax= 2.53D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 4.17D-05 CP: 1.00D+00 1.05D+00

E= -1658.67690871800 Delta-E= -0.000046495659 Rises=F Damp=F

DIIS: error= 2.81D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67690871800 IErMin= 2 ErrMin= 2.50D-04

ErrMax= 2.81D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.21D-04 BMatP= 1.97D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 2.81D-03

Coeff-Com: -0.355D-01 0.493D+00 0.543D+00

Coeff-En: 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.354D-01 0.492D+00 0.544D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=2.74D-05 MaxDP=1.22D-03 DE=-4.65D-05 OVMax= 2.86D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.02D-05 CP: 1.00D+00 1.08D+00 6.08D-01

E= -1658.67692824231 Delta-E= -0.000019524308 Rises=F Damp=F

DIIS: error= 1.78D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67692824231 IErMin= 4 ErrMin= 1.78D-04

ErrMax= 1.78D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.10D-05 BMatP= 1.21D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.78D-03

Coeff-Com: -0.131D-01 0.167D+00 0.369D+00 0.477D+00

Coeff-En: 0.000D+00 0.000D+00 0.267D+00 0.733D+00

Coeff: -0.130D-01 0.166D+00 0.369D+00 0.478D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.10D-05 MaxDP=4.70D-04 DE=-1.95D-05 OVMax= 1.02D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 6.69D-06 CP: 1.00D+00 1.09D+00 6.91D-01 6.13D-01

E= -1658.67693764748 Delta-E= -0.000009405170 Rises=F Damp=F

DIIS: error= 3.54D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67693764748 IErMin= 5 ErrMin= 3.54D-05

ErrMax= 3.54D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.30D-06 BMatP= 4.10D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.295D-02 0.314D-01 0.129D+00 0.220D+00 0.623D+00

Coeff: -0.295D-02 0.314D-01 0.129D+00 0.220D+00 0.623D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.66D-06 MaxDP=9.23D-05 DE=-9.41D-06 OVMax= 2.32D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.85D-06 CP: 1.00D+00 1.09D+00 7.08D-01 6.97D-01 9.19D-01

E= -1658.67693792204 Delta-E= -0.000000274556 Rises=F Damp=F

DIIS: error= 2.23D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67693792204 IErMin= 6 ErrMin= 2.23D-05

ErrMax= 2.23D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.25D-07 BMatP= 1.30D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.999D-03-0.183D-01 0.400D-02 0.390D-01 0.394D+00 0.580D+00

Coeff: 0.999D-03-0.183D-01 0.400D-02 0.390D-01 0.394D+00 0.580D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.23D-06 MaxDP=4.75D-05 DE=-2.75D-07 OVMax= 1.43D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 8.53D-07 CP: 1.00D+00 1.09D+00 7.22D-01 7.17D-01 9.91D-01

CP: 8.64D-01

E= -1658.67693802263 Delta-E= -0.000000100598 Rises=F Damp=F

DIIS: error= 5.08D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67693802263 IErMin= 7 ErrMin= 5.08D-06

ErrMax= 5.08D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.97D-08 BMatP= 4.25D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.643D-03-0.941D-02-0.120D-01-0.111D-01 0.622D-01 0.195D+00

Coeff-Com: 0.775D+00

Coeff: 0.643D-03-0.941D-02-0.120D-01-0.111D-01 0.622D-01 0.195D+00

Coeff: 0.775D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.55D-07 MaxDP=2.27D-05 DE=-1.01D-07 OVMax= 7.90D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 3.14D-07 CP: 1.00D+00 1.09D+00 7.24D-01 7.25D-01 1.04D+00

CP: 9.67D-01 1.20D+00

E= -1658.67693802973 Delta-E= -0.000000007097 Rises=F Damp=F

DIIS: error= 3.87D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67693802973 IErMin= 8 ErrMin= 3.87D-06

ErrMax= 3.87D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.10D-08 BMatP= 1.97D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.200D-03-0.214D-02-0.804D-02-0.146D-01-0.376D-01 0.964D-02

Coeff-Com: 0.484D+00 0.569D+00

Coeff: 0.200D-03-0.214D-02-0.804D-02-0.146D-01-0.376D-01 0.964D-02

Coeff: 0.484D+00 0.569D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.87D-07 MaxDP=1.01D-05 DE=-7.10D-09 OVMax= 3.70D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.50D-07 CP: 1.00D+00 1.09D+00 7.24D-01 7.31D-01 1.05D+00

CP: 1.03D+00 1.35D+00 8.35D-01

E= -1658.67693803268 Delta-E= -0.000000002947 Rises=F Damp=F

DIIS: error= 1.41D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67693803268 IErMin= 9 ErrMin= 1.41D-06

ErrMax= 1.41D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.94D-09 BMatP= 1.10D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.304D-04 0.989D-03-0.219D-02-0.658D-02-0.380D-01-0.394D-01

Coeff-Com: 0.107D+00 0.341D+00 0.637D+00

Coeff: -0.304D-04 0.989D-03-0.219D-02-0.658D-02-0.380D-01-0.394D-01

Coeff: 0.107D+00 0.341D+00 0.637D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.26D-07 MaxDP=4.81D-06 DE=-2.95D-09 OVMax= 1.87D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 5.67D-08 CP: 1.00D+00 1.09D+00 7.25D-01 7.32D-01 1.05D+00

CP: 1.06D+00 1.43D+00 9.54D-01 7.88D-01

E= -1658.67693803319 Delta-E= -0.000000000516 Rises=F Damp=F

DIIS: error= 3.48D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67693803319 IErMin=10 ErrMin= 3.48D-07

ErrMax= 3.48D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.99D-10 BMatP= 1.94D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.458D-04 0.876D-03-0.113D-03-0.162D-02-0.157D-01-0.232D-01

Coeff-Com: -0.133D-01 0.107D+00 0.361D+00 0.586D+00

Coeff: -0.458D-04 0.876D-03-0.113D-03-0.162D-02-0.157D-01-0.232D-01

Coeff: -0.133D-01 0.107D+00 0.361D+00 0.586D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.35D-08 MaxDP=1.72D-06 DE=-5.16D-10 OVMax= 4.86D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 2.15D-08 CP: 1.00D+00 1.09D+00 7.25D-01 7.33D-01 1.05D+00

CP: 1.06D+00 1.45D+00 9.97D-01 9.03D-01 7.87D-01

E= -1658.67693803333 Delta-E= -0.000000000136 Rises=F Damp=F

DIIS: error= 5.93D-08 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67693803333 IErMin=11 ErrMin= 5.93D-08

ErrMax= 5.93D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.32D-11 BMatP= 2.99D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.989D-05 0.140D-03 0.182D-03 0.245D-03-0.174D-03-0.204D-02

Coeff-Com: -0.162D-01-0.722D-02 0.340D-01 0.179D+00 0.812D+00

Coeff: -0.989D-05 0.140D-03 0.182D-03 0.245D-03-0.174D-03-0.204D-02

Coeff: -0.162D-01-0.722D-02 0.340D-01 0.179D+00 0.812D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.59D-08 MaxDP=6.33D-07 DE=-1.36D-10 OVMax= 1.81D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 8.97D-09 CP: 1.00D+00 1.09D+00 7.25D-01 7.33D-01 1.05D+00

CP: 1.07D+00 1.46D+00 1.01D+00 9.46D-01 9.16D-01

CP: 1.02D+00

E= -1658.67693803331 Delta-E= 0.000000000017 Rises=F Damp=F

DIIS: error= 3.10D-08 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=11 EnMin= -1658.67693803333 IErMin=12 ErrMin= 3.10D-08

ErrMax= 3.10D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.80D-12 BMatP= 1.32D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.177D-05-0.603D-04 0.992D-04 0.346D-03 0.216D-02 0.245D-02

Coeff-Com: -0.589D-02-0.195D-01-0.357D-01 0.104D-02 0.393D+00 0.662D+00

Coeff: 0.177D-05-0.603D-04 0.992D-04 0.346D-03 0.216D-02 0.245D-02

Coeff: -0.589D-02-0.195D-01-0.357D-01 0.104D-02 0.393D+00 0.662D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.89D-09 MaxDP=2.70D-07 DE= 1.68D-11 OVMax= 5.53D-07

Error on total polarization charges = 0.04169

SCF Done: E(UB3LYP) = -1658.67693803 A.U. after 12 cycles

NFock= 12 Conv=0.59D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655251261120D+03 PE=-6.146480236725D+03 EE= 1.730699206975D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.61

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:37:02 2019, MaxMem= 1342177280 cpu: 298.9

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 338

Leave Link 701 at Sat Aug 17 17:37:03 2019, MaxMem= 1342177280 cpu: 10.3

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:37:03 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:37:06 2019, MaxMem= 1342177280 cpu: 36.1

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.37330530D+00-2.91853495D+00 5.86770619D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.001898925 -0.001029469 -0.000010374

2 6 -0.000308698 -0.000188446 0.000588917

3 8 -0.001553767 0.001348723 -0.000709033

4 8 0.000070792 -0.000355266 0.000432518

5 6 0.000178798 -0.000116469 0.000110202

6 16 0.000179582 0.000365653 -0.000389476

7 6 -0.000126206 -0.000079262 -0.000127397

8 16 0.000302296 -0.000144001 0.000217531

9 16 -0.000072103 0.000065846 0.000090875

10 6 -0.000322495 -0.000111959 -0.000005004

11 6 0.000024847 -0.000053303 -0.000024415

12 6 -0.000109968 0.000034349 -0.000153966

13 6 0.000121218 -0.000131096 0.000039217

14 1 -0.000119806 0.000221188 0.000184960

15 1 -0.000299611 -0.000019864 -0.000190278

16 1 0.000223379 0.000039907 0.000095783

17 1 -0.000143905 0.000030084 0.000062794

18 1 -0.000049120 -0.000179456 -0.000086320

19 1 0.000245465 0.000314734 -0.000268706

20 1 -0.000180620 -0.000012010 0.000312528

21 1 -0.000080849 -0.000003330 0.000139724

22 1 0.000093653 -0.000150363 -0.000219393

23 1 -0.000004162 0.000128445 -0.000125190

24 1 0.000018268 0.000023163 0.000187406

25 1 0.000132823 0.000112134 -0.000020114

26 1 -0.000021948 -0.000124959 0.000113282

27 1 -0.000096789 0.000015027 -0.000246071

-------------------------------------------------------------------

Cartesian Forces: Max 0.001898925 RMS 0.000384857

Leave Link 716 at Sat Aug 17 17:37:06 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.002147776 RMS 0.000244158

Search for a local minimum.

Step number 17 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .24416D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

DE= -2.99D-05 DEPred=-3.38D-05 R= 8.87D-01

TightC=F SS= 1.41D+00 RLast= 1.51D-01 DXNew= 1.6818D-01 4.5306D-01

Trust test= 8.87D-01 RLast= 1.51D-01 DXMaxT set to 1.68D-01

ITU= 1 1 -1 1 -1 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Eigenvalues --- 0.00034 0.00197 0.00297 0.00377 0.00428

Eigenvalues --- 0.00525 0.00740 0.01013 0.01534 0.02333

Eigenvalues --- 0.02510 0.03264 0.03546 0.03761 0.04608

Eigenvalues --- 0.04805 0.04833 0.05102 0.05268 0.05461

Eigenvalues --- 0.05463 0.05643 0.05818 0.05892 0.08232

Eigenvalues --- 0.08275 0.08378 0.11338 0.12197 0.12259

Eigenvalues --- 0.14122 0.15379 0.15925 0.16001 0.16031

Eigenvalues --- 0.16062 0.16272 0.16475 0.17827 0.18461

Eigenvalues --- 0.21479 0.21962 0.21972 0.23194 0.23301

Eigenvalues --- 0.24255 0.24743 0.25416 0.25940 0.27015

Eigenvalues --- 0.27888 0.29106 0.29431 0.29648 0.29856

Eigenvalues --- 0.30370 0.31390 0.32820 0.33853 0.33868

Eigenvalues --- 0.33881 0.33908 0.33965 0.34033 0.34060

Eigenvalues --- 0.34131 0.34224 0.34483 0.34548 0.34594

Eigenvalues --- 0.34778 0.41722 0.52627 0.59659 1.50980

En-DIIS/RFO-DIIS IScMMF= 0 using points: 17 16 15 14 13

RFO step: Lambda=-1.03437585D-05.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 2.53D-05 SmlDif= 1.00D-05

RMS Error= 0.1105734407D-02 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.13151 1.53584 -1.35523 0.08681 -0.39892

Iteration 1 RMS(Cart)= 0.15821381 RMS(Int)= 0.00611149

Iteration 2 RMS(Cart)= 0.02222461 RMS(Int)= 0.00007585

Iteration 3 RMS(Cart)= 0.00017758 RMS(Int)= 0.00005632

Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00005632

ITry= 1 IFail=0 DXMaxC= 5.78D-01 DCOld= 1.00D+10 DXMaxT= 1.68D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83745 0.00014 -0.00137 -0.00145 -0.00282 2.83463

R2 2.28578 0.00215 -0.00235 0.00097 -0.00138 2.28441

R3 2.55261 0.00045 -0.00087 0.00082 -0.00005 2.55255

R4 2.86635 0.00026 -0.00057 -0.00072 -0.00130 2.86505

R5 3.59415 0.00044 -0.00029 0.00908 0.00879 3.60294

R6 2.05714 0.00028 -0.00094 -0.00019 -0.00113 2.05601

R7 1.83622 0.00034 -0.00099 -0.00019 -0.00117 1.83504

R8 2.06088 0.00025 -0.00085 -0.00134 -0.00218 2.05870

R9 2.06843 0.00015 -0.00079 -0.00078 -0.00157 2.06686

R10 2.05983 0.00014 -0.00068 -0.00021 -0.00088 2.05895

R11 3.32156 -0.00015 -0.00043 -0.00140 -0.00182 3.31973

R12 3.38396 0.00023 0.00071 0.00088 0.00159 3.38555

R13 3.25377 0.00007 -0.00082 0.00017 -0.00065 3.25312

R14 3.47552 -0.00015 -0.00098 -0.00304 -0.00403 3.47149

R15 2.88061 0.00020 -0.00067 -0.00049 -0.00115 2.87946

R16 2.06311 0.00040 -0.00114 -0.00022 -0.00136 2.06175

R17 2.05966 0.00021 -0.00087 -0.00037 -0.00124 2.05842

R18 2.89381 0.00005 -0.00038 0.00043 0.00005 2.89386

R19 2.07197 0.00014 -0.00059 0.00028 -0.00031 2.07166

R20 2.07042 0.00025 -0.00071 0.00009 -0.00062 2.06980

R21 2.88557 0.00020 -0.00066 -0.00071 -0.00136 2.88421

R22 2.07151 0.00017 -0.00064 0.00004 -0.00061 2.07091

R23 2.07132 0.00016 -0.00060 0.00022 -0.00038 2.07094

R24 2.06725 0.00017 -0.00064 -0.00004 -0.00067 2.06657

R25 2.06871 0.00019 -0.00067 0.00019 -0.00048 2.06823

R26 2.06855 0.00017 -0.00063 0.00002 -0.00061 2.06794

A1 2.17825 -0.00002 0.00092 -0.00206 -0.00114 2.17711

A2 1.97413 0.00004 -0.00131 0.00126 -0.00005 1.97408

A3 2.13012 -0.00001 0.00065 0.00029 0.00094 2.13106

A4 2.02140 0.00014 0.00119 0.00393 0.00511 2.02651

A5 1.84068 -0.00027 0.00111 -0.00348 -0.00236 1.83832

A6 1.87175 0.00005 0.00207 0.00296 0.00504 1.87679

A7 1.94572 0.00018 -0.00330 -0.00505 -0.00835 1.93737

A8 1.94013 -0.00013 -0.00097 -0.00377 -0.00476 1.93537

A9 1.83165 0.00002 0.00004 0.00594 0.00595 1.83760

A10 1.87410 -0.00004 0.00007 0.00133 0.00140 1.87549

A11 1.91156 0.00004 -0.00160 -0.00535 -0.00694 1.90461

A12 1.92904 -0.00017 0.00154 0.00028 0.00182 1.93086

A13 1.95238 0.00000 0.00025 0.00194 0.00218 1.95456

A14 1.88326 0.00004 0.00005 0.00186 0.00192 1.88518

A15 1.89338 0.00002 -0.00029 0.00122 0.00093 1.89431

A16 1.89256 0.00006 0.00003 0.00014 0.00016 1.89272

A17 1.79224 -0.00028 -0.00124 0.00421 0.00297 1.79521

A18 1.97008 -0.00011 -0.00330 -0.00563 -0.00928 1.96080

A19 2.14277 -0.00010 -0.00002 -0.00097 -0.00134 2.14143

A20 2.15388 0.00017 0.00122 0.00146 0.00231 2.15619

A21 1.79431 0.00030 0.00180 0.00431 0.00611 1.80043

A22 1.92669 -0.00032 0.00009 -0.00265 -0.00255 1.92414

A23 1.87412 0.00036 -0.00126 -0.00097 -0.00223 1.87190

A24 1.89641 -0.00012 0.00055 -0.00049 0.00006 1.89647

A25 1.93922 -0.00012 0.00095 0.00249 0.00344 1.94266

A26 1.93861 0.00019 -0.00015 0.00114 0.00098 1.93959

A27 1.88684 0.00001 -0.00022 0.00041 0.00019 1.88703

A28 1.95360 0.00012 0.00009 0.00093 0.00102 1.95462

A29 1.91794 -0.00013 0.00021 0.00027 0.00048 1.91842

A30 1.91455 0.00006 0.00007 -0.00032 -0.00025 1.91430

A31 1.90605 0.00002 -0.00028 0.00038 0.00010 1.90615

A32 1.91016 -0.00013 0.00067 -0.00012 0.00055 1.91071

A33 1.85912 0.00004 -0.00080 -0.00125 -0.00205 1.85707

A34 1.96675 -0.00011 0.00019 -0.00029 -0.00011 1.96664

A35 1.90642 0.00005 0.00046 0.00002 0.00047 1.90690

A36 1.90762 0.00001 -0.00015 0.00070 0.00055 1.90817

A37 1.91266 0.00002 0.00070 0.00077 0.00147 1.91413

A38 1.91290 0.00004 -0.00057 -0.00093 -0.00150 1.91140

A39 1.85407 0.00000 -0.00068 -0.00026 -0.00094 1.85313

A40 1.94556 0.00000 0.00021 0.00026 0.00047 1.94603

A41 1.94256 0.00000 -0.00002 -0.00076 -0.00077 1.94179

A42 1.94383 -0.00017 0.00100 0.00156 0.00256 1.94639

A43 1.87612 0.00002 -0.00018 0.00057 0.00040 1.87651

A44 1.87677 0.00007 -0.00034 0.00008 -0.00026 1.87651

A45 1.87551 0.00009 -0.00076 -0.00179 -0.00256 1.87296

D1 2.64180 -0.00017 0.00193 0.07693 0.07887 2.72067

D2 -1.48112 -0.00006 -0.00068 0.07032 0.06963 -1.41149

D3 0.46443 -0.00014 0.00071 0.07672 0.07741 0.54184

D4 -0.53925 0.00017 0.00981 0.06241 0.07224 -0.46700

D5 1.62102 0.00028 0.00720 0.05581 0.06300 1.68402

D6 -2.71661 0.00021 0.00859 0.06221 0.07078 -2.64583

D7 -3.10300 -0.00018 -0.00213 0.01168 0.00956 -3.09344

D8 0.00037 0.00015 0.00553 -0.00244 0.00308 0.00345

D9 -3.11761 -0.00006 0.00618 0.00987 0.01606 -3.10156

D10 -1.04499 -0.00008 0.00619 0.00901 0.01521 -1.02978

D11 1.06573 -0.00012 0.00746 0.01069 0.01816 1.08389

D12 1.06112 0.00005 0.00643 0.01562 0.02206 1.08318

D13 3.13374 0.00003 0.00644 0.01476 0.02121 -3.12823

D14 -1.03872 0.00000 0.00771 0.01644 0.02416 -1.01456

D15 -0.97592 0.00000 0.00910 0.01380 0.02289 -0.95304

D16 1.09670 -0.00002 0.00911 0.01294 0.02204 1.11874

D17 -3.07577 -0.00006 0.01038 0.01462 0.02499 -3.05078

D18 3.14064 0.00013 0.03423 0.06802 0.10224 -3.04031

D19 -0.93515 0.00023 0.03439 0.06730 0.10172 -0.83343

D20 1.16685 0.00018 0.03145 0.06368 0.09512 1.26196

D21 1.84728 -0.00021 -0.01388 -0.05814 -0.07195 1.77533

D22 -1.10623 0.00002 -0.00087 -0.02924 -0.03018 -1.13640

D23 2.54873 0.00025 0.04367 0.09362 0.13728 2.68601

D24 -0.78233 -0.00002 0.03043 0.06419 0.09462 -0.68770

D25 -3.01409 0.00006 -0.03495 -0.07223 -0.10718 -3.12127

D26 -0.89768 -0.00004 -0.03452 -0.07137 -0.10588 -1.00356

D27 1.13922 0.00010 -0.03517 -0.07165 -0.10682 1.03240

D28 -3.10623 0.00010 0.00433 0.00142 0.00575 -3.10048

D29 -0.98523 0.00013 0.00418 0.00272 0.00690 -0.97833

D30 1.05309 0.00014 0.00337 0.00118 0.00454 1.05764

D31 1.09970 -0.00007 0.00523 0.00275 0.00799 1.10768

D32 -3.06249 -0.00005 0.00508 0.00405 0.00914 -3.05335

D33 -1.02417 -0.00003 0.00427 0.00251 0.00678 -1.01739

D34 -1.00142 -0.00013 0.00498 -0.00021 0.00476 -0.99666

D35 1.11958 -0.00011 0.00483 0.00108 0.00591 1.12549

D36 -3.12529 -0.00009 0.00402 -0.00046 0.00356 -3.12173

D37 -3.12454 -0.00003 -0.01314 -0.01565 -0.02880 3.12985

D38 -0.99438 -0.00004 -0.01180 -0.01486 -0.02666 -1.02103

D39 1.02733 -0.00001 -0.01244 -0.01476 -0.02721 1.00012

D40 1.03081 0.00004 -0.01327 -0.01688 -0.03015 1.00066

D41 -3.12221 0.00002 -0.01193 -0.01608 -0.02801 3.13297

D42 -1.10051 0.00006 -0.01257 -0.01599 -0.02856 -1.12906

D43 -0.99816 0.00005 -0.01253 -0.01553 -0.02805 -1.02621

D44 1.13201 0.00003 -0.01118 -0.01473 -0.02591 1.10609

D45 -3.12947 0.00007 -0.01183 -0.01464 -0.02646 3.12725

D46 -3.14087 0.00000 -0.00283 -0.01681 -0.01964 3.12268

D47 -1.04639 0.00003 -0.00292 -0.01642 -0.01934 -1.06573

D48 1.04615 0.00003 -0.00323 -0.01815 -0.02138 1.02478

D49 1.01568 0.00000 -0.00404 -0.01718 -0.02122 0.99446

D50 3.11016 0.00003 -0.00414 -0.01679 -0.02092 3.08923

D51 -1.08049 0.00003 -0.00444 -0.01852 -0.02296 -1.10345

D52 -1.01253 -0.00003 -0.00330 -0.01678 -0.02007 -1.03260

D53 1.08195 0.00000 -0.00339 -0.01639 -0.01977 1.06217

D54 -3.10869 0.00000 -0.00369 -0.01812 -0.02181 -3.13051

Item Value Threshold Converged?

Maximum Force 0.002148 0.000450 NO

RMS Force 0.000244 0.000300 YES

Maximum Displacement 0.578497 0.001800 NO

RMS Displacement 0.167525 0.001200 NO

Predicted change in Energy=-6.209752D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:37:06 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.089349 -0.464484 -0.100981

2 6 0 -2.819557 0.082689 0.480650

3 8 0 -4.957697 0.204284 -0.610934

4 8 0 -4.156078 -1.812769 -0.053976

5 6 0 -2.147330 -0.771555 1.537533

6 16 0 -1.662779 0.363096 -1.008760

7 6 0 -0.151963 0.835385 -0.246877

8 16 0 1.032875 -0.507366 -0.193513

9 16 0 0.018919 2.291136 0.655938

10 6 0 2.649796 0.363338 -0.147294

11 6 0 3.791549 -0.645528 -0.127747

12 6 0 5.158721 0.037488 -0.030718

13 6 0 6.313493 -0.959796 0.006525

14 1 0 -3.037181 1.076628 0.865947

15 1 0 -4.983152 -2.078813 -0.487721

16 1 0 -1.264700 -0.251684 1.908387

17 1 0 -2.820822 -0.939788 2.382732

18 1 0 -1.839275 -1.739801 1.144189

19 1 0 2.699307 1.000986 -1.031205

20 1 0 2.676018 1.003166 0.733866

21 1 0 3.669774 -1.330987 0.719089

22 1 0 3.754666 -1.261930 -1.032374

23 1 0 5.284830 0.716306 -0.881747

24 1 0 5.187819 0.664988 0.867269

25 1 0 7.280514 -0.451572 0.056590

26 1 0 6.241620 -1.617717 0.878201

27 1 0 6.322141 -1.597337 -0.882844

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.500021 0.000000

3 O 1.208855 2.403743 0.000000

4 O 1.350754 2.380100 2.240825 0.000000

5 C 2.559386 1.516121 3.669650 2.766242 0.000000

6 S 2.719778 1.906596 3.322645 3.444205 2.829458

7 C 4.148970 2.865643 4.860648 4.804464 3.122158

8 S 5.123238 3.955236 6.047117 5.352456 3.630430

9 S 5.004421 3.600682 5.543159 5.897170 3.853560

10 C 6.789957 5.512432 7.623268 7.145914 5.209515

11 C 7.883022 6.678860 8.803690 8.033223 6.169224

12 C 9.261949 7.994777 10.134415 9.496814 7.516139

13 C 10.415182 9.204574 11.347954 10.504435 8.600288

14 H 2.101674 1.087993 2.574984 3.232152 2.158389

15 H 1.885341 3.207955 2.286561 0.971064 3.721890

16 H 3.472964 2.137246 4.493674 3.827261 1.089419

17 H 2.829117 2.159485 3.851905 2.912483 1.093734

18 H 2.870490 2.173179 4.072404 2.609311 1.089549

19 H 7.007051 5.795416 7.709803 7.474524 5.764565

20 H 6.972887 5.577880 7.792323 7.431536 5.201943

21 H 7.850307 6.645807 8.863367 7.878687 5.900976

22 H 7.939268 6.878783 8.844923 7.990029 6.455885

23 H 9.480458 8.242493 10.258892 9.808781 7.956360

24 H 9.395693 8.037824 10.262983 9.710633 7.504487

25 H 11.370962 10.123077 12.273937 11.517844 9.548813

26 H 10.441152 9.227912 11.443859 10.441223 8.457257

27 H 10.502085 9.394267 11.426046 10.513160 8.847152

6 7 8 9 10

6 S 0.000000

7 C 1.756726 0.000000

8 S 2.947690 1.791555 0.000000

9 S 3.052321 1.721478 3.095365 0.000000

10 C 4.397776 2.842992 1.837035 3.359033 0.000000

11 C 5.616333 4.214093 2.762915 4.844677 1.523742

12 C 6.898945 5.374638 4.164850 5.654024 2.532680

13 C 8.148728 6.714836 5.303739 7.114209 3.898335

14 H 2.431591 3.101783 4.494089 3.295281 5.820408

15 H 4.154429 5.647207 6.224836 6.739817 8.021340

16 H 3.007685 2.658020 3.124453 3.111630 4.464007

17 H 3.813238 4.145949 4.655642 4.635171 6.166590

18 H 3.014717 3.378413 3.399645 4.465392 5.122781

19 H 4.408537 2.961813 2.398718 3.419857 1.091029

20 H 4.719279 2.997914 2.416952 2.953831 1.089271

21 H 5.855895 4.497992 2.909370 5.143200 2.159100

22 H 5.655968 4.503053 2.946388 5.424987 2.155365

23 H 6.957741 5.475030 4.477741 5.707397 2.758153

24 H 7.109241 5.457438 4.445586 5.422780 2.749889

25 H 9.043292 7.549176 6.252892 7.785398 4.706293

26 H 8.364434 6.939843 5.432539 7.351907 4.228169

27 H 8.223023 6.945259 5.444222 7.564303 4.227457

11 12 13 14 15

11 C 0.000000

12 C 1.531367 0.000000

13 C 2.544995 1.526258 0.000000

14 H 7.112299 8.310031 9.608368 0.000000

15 H 8.898274 10.370399 11.362688 3.946648 0.000000

16 H 5.465035 6.715958 7.845223 2.448016 4.786086

17 H 7.079021 8.393623 9.438351 2.532465 3.769954

18 H 5.875494 7.315129 8.268635 3.073217 3.558374

19 H 2.172610 2.824539 4.240742 6.042533 8.294620

20 H 2.169095 2.771450 4.196840 5.715198 8.345883

21 H 1.096273 2.156826 2.763111 7.127511 8.768624

22 H 1.095291 2.159438 2.778163 7.429782 8.792805

23 H 2.157081 1.095878 2.157891 8.511177 10.648916

24 H 2.158026 1.095894 2.155910 8.235294 10.621351

25 H 3.499210 2.179176 1.093584 10.461609 12.383121

26 H 2.821335 2.176811 1.094461 9.662080 11.316972

27 H 2.807136 2.179981 1.094307 9.889654 11.322438

16 17 18 19 20

16 H 0.000000

17 H 1.766353 0.000000

18 H 1.768792 1.771283 0.000000

19 H 5.091536 6.774466 5.730879 0.000000

20 H 4.299234 6.058802 5.299066 1.765226 0.000000

21 H 5.189254 6.711824 5.540529 3.073017 2.536935

22 H 5.904465 7.416452 6.021459 2.496912 3.068182

23 H 7.184581 8.893878 7.803189 2.605438 3.081946

24 H 6.599941 8.307241 7.432344 3.147981 2.537972

25 H 8.745844 10.377199 9.274317 4.927543 4.876099

26 H 7.698842 9.211463 8.086193 4.801189 4.427570

27 H 8.195237 9.730885 8.410581 4.460742 4.761363

21 22 23 24 25

21 H 0.000000

22 H 1.754878 0.000000

23 H 3.059819 2.505496 0.000000

24 H 2.512038 3.061957 1.752456 0.000000

25 H 3.774880 3.778111 2.495430 2.506647 0.000000

26 H 2.592667 3.156235 3.075797 2.514232 1.764720

27 H 3.110013 2.593605 2.535539 3.076962 1.764593

26 27

26 H 0.000000

27 H 1.763002 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 5.88D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.080669 -0.504509 -0.032338

2 6 0 -2.807289 0.091630 0.490334

3 8 0 -4.949569 0.115580 -0.599641

4 8 0 -4.150255 -1.842205 0.141622

5 6 0 -2.132703 -0.661120 1.620345

6 16 0 -1.655946 0.227568 -1.023283

7 6 0 -0.140980 0.765486 -0.315037

8 16 0 1.041026 -0.569398 -0.140067

9 16 0 0.036862 2.299289 0.446084

10 6 0 2.660086 0.297530 -0.182211

11 6 0 3.799625 -0.708021 -0.072169

12 6 0 5.168721 -0.022508 -0.045105

13 6 0 6.321378 -1.014898 0.081413

14 1 0 -3.021096 1.117989 0.781197

15 1 0 -4.979685 -2.145712 -0.261980

16 1 0 -1.247399 -0.110980 1.937231

17 1 0 -2.803131 -0.747285 2.480203

18 1 0 -1.828440 -1.662896 1.318705

19 1 0 2.707444 0.849025 -1.122400

20 1 0 2.691338 1.017377 0.634706

21 1 0 3.679745 -1.310415 0.835886

22 1 0 3.757671 -1.406728 -0.914613

23 1 0 5.292903 0.572867 -0.956727

24 1 0 5.202889 0.686643 0.789713

25 1 0 7.289740 -0.506767 0.079710

26 1 0 6.251562 -1.587669 1.011415

27 1 0 6.324968 -1.733333 -0.744025

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2864906 0.1963866 0.1828578

Leave Link 202 at Sat Aug 17 17:37:06 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1105.5858680051 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0553623645 Hartrees.

Nuclear repulsion after empirical dispersion term = 1105.5305056406 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

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Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2330

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.68D-11

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 109

GePol: Fraction of low-weight points (<1% of avg) = 4.68%

GePol: Cavity surface area = 306.415 Ang\*\*2

GePol: Cavity volume = 319.471 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0056198212 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1105.5248858194 Hartrees.

Leave Link 301 at Sat Aug 17 17:37:06 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:37:06 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:37:06 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999696 -0.024402 -0.003497 -0.000428 Ang= -2.83 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.63092476475

Leave Link 401 at Sat Aug 17 17:37:07 2019, MaxMem= 1342177280 cpu: 7.5

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16286700.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.22D-15 for 2314.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.41D-15 for 684 329.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.44D-15 for 2314.

Iteration 1 A^-1\*A deviation from orthogonality is 4.64D-11 for 1291 1163.

E= -1658.63847871760

DIIS: error= 6.82D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.63847871760 IErMin= 1 ErrMin= 6.82D-03

ErrMax= 6.82D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.93D-02 BMatP= 7.93D-02

IDIUse=3 WtCom= 9.32D-01 WtEn= 6.82D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.429 Goal= None Shift= 0.000

Gap= 0.486 Goal= None Shift= 0.000

GapD= 0.429 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=7.58D-04 MaxDP=2.77D-02 OVMax= 4.80D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 7.58D-04 CP: 9.98D-01

E= -1658.67608853071 Delta-E= -0.037609813114 Rises=F Damp=F

DIIS: error= 8.62D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67608853071 IErMin= 2 ErrMin= 8.62D-04

ErrMax= 8.62D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.49D-03 BMatP= 7.93D-02

IDIUse=3 WtCom= 9.91D-01 WtEn= 8.62D-03

Coeff-Com: -0.591D-01 0.106D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.586D-01 0.106D+01

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=1.27D-04 MaxDP=4.25D-03 DE=-3.76D-02 OVMax= 7.52D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.23D-04 CP: 9.98D-01 1.04D+00

E= -1658.67642635023 Delta-E= -0.000337819512 Rises=F Damp=F

DIIS: error= 8.16D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67642635023 IErMin= 3 ErrMin= 8.16D-04

ErrMax= 8.16D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.79D-04 BMatP= 1.49D-03

IDIUse=3 WtCom= 9.92D-01 WtEn= 8.16D-03

Coeff-Com: -0.355D-01 0.498D+00 0.538D+00

Coeff-En: 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.352D-01 0.493D+00 0.542D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=7.40D-05 MaxDP=3.03D-03 DE=-3.38D-04 OVMax= 7.60D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 5.43D-05 CP: 9.98D-01 1.08D+00 6.59D-01

E= -1658.67659567666 Delta-E= -0.000169326438 Rises=F Damp=F

DIIS: error= 4.86D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67659567666 IErMin= 4 ErrMin= 4.86D-04

ErrMax= 4.86D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.58D-04 BMatP= 9.79D-04

IDIUse=3 WtCom= 9.95D-01 WtEn= 4.86D-03

Coeff-Com: -0.135D-01 0.174D+00 0.351D+00 0.489D+00

Coeff-En: 0.000D+00 0.000D+00 0.207D+00 0.793D+00

Coeff: -0.135D-01 0.173D+00 0.350D+00 0.491D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=2.87D-05 MaxDP=1.18D-03 DE=-1.69D-04 OVMax= 2.66D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.98D-05 CP: 9.98D-01 1.09D+00 7.20D-01 6.63D-01

E= -1658.67665271952 Delta-E= -0.000057042860 Rises=F Damp=F

DIIS: error= 7.93D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67665271952 IErMin= 5 ErrMin= 7.93D-05

ErrMax= 7.93D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.21D-05 BMatP= 2.58D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.350D-02 0.388D-01 0.132D+00 0.246D+00 0.586D+00

Coeff: -0.350D-02 0.388D-01 0.132D+00 0.246D+00 0.586D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=8.60D-06 MaxDP=3.52D-04 DE=-5.70D-05 OVMax= 1.01D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 5.57D-06 CP: 9.98D-01 1.09D+00 7.35D-01 7.72D-01 8.95D-01

E= -1658.67665541101 Delta-E= -0.000002691489 Rises=F Damp=F

DIIS: error= 5.06D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67665541101 IErMin= 6 ErrMin= 5.06D-05

ErrMax= 5.06D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.34D-06 BMatP= 1.21D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.962D-03-0.181D-01 0.521D-02 0.455D-01 0.372D+00 0.594D+00

Coeff: 0.962D-03-0.181D-01 0.521D-02 0.455D-01 0.372D+00 0.594D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=4.01D-06 MaxDP=1.51D-04 DE=-2.69D-06 OVMax= 4.71D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.53D-06 CP: 9.98D-01 1.09D+00 7.53D-01 7.88D-01 9.85D-01

CP: 8.66D-01

E= -1658.67665628124 Delta-E= -0.000000870226 Rises=F Damp=F

DIIS: error= 1.38D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67665628124 IErMin= 7 ErrMin= 1.38D-05

ErrMax= 1.38D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.62D-07 BMatP= 3.34D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.708D-03-0.104D-01-0.117D-01-0.113D-01 0.647D-01 0.206D+00

Coeff-Com: 0.762D+00

Coeff: 0.708D-03-0.104D-01-0.117D-01-0.113D-01 0.647D-01 0.206D+00

Coeff: 0.762D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=1.76D-06 MaxDP=7.08D-05 DE=-8.70D-07 OVMax= 2.44D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 9.91D-07 CP: 9.98D-01 1.09D+00 7.56D-01 8.03D-01 1.03D+00

CP: 9.72D-01 1.16D+00

E= -1658.67665634964 Delta-E= -0.000000068397 Rises=F Damp=F

DIIS: error= 9.44D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67665634964 IErMin= 8 ErrMin= 9.44D-06

ErrMax= 9.44D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.84D-08 BMatP= 1.62D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.165D-03-0.150D-02-0.676D-02-0.152D-01-0.409D-01-0.150D-01

Coeff-Com: 0.405D+00 0.674D+00

Coeff: 0.165D-03-0.150D-02-0.676D-02-0.152D-01-0.409D-01-0.150D-01

Coeff: 0.405D+00 0.674D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=8.83D-07 MaxDP=3.66D-05 DE=-6.84D-08 OVMax= 1.35D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 4.01D-07 CP: 9.98D-01 1.09D+00 7.57D-01 8.10D-01 1.04D+00

CP: 1.04D+00 1.33D+00 9.97D-01

E= -1658.67665636822 Delta-E= -0.000000018588 Rises=F Damp=F

DIIS: error= 5.15D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67665636822 IErMin= 9 ErrMin= 5.15D-06

ErrMax= 5.15D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.58D-08 BMatP= 5.84D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.213D-04 0.907D-03-0.230D-02-0.787D-02-0.365D-01-0.458D-01

Coeff-Com: 0.111D+00 0.413D+00 0.567D+00

Coeff: -0.213D-04 0.907D-03-0.230D-02-0.787D-02-0.365D-01-0.458D-01

Coeff: 0.111D+00 0.413D+00 0.567D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=3.29D-07 MaxDP=1.02D-05 DE=-1.86D-08 OVMax= 4.51D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.72D-07 CP: 9.98D-01 1.09D+00 7.58D-01 8.11D-01 1.04D+00

CP: 1.05D+00 1.40D+00 1.06D+00 7.57D-01

E= -1658.67665637206 Delta-E= -0.000000003838 Rises=F Damp=F

DIIS: error= 2.08D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67665637206 IErMin=10 ErrMin= 2.08D-06

ErrMax= 2.08D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.96D-09 BMatP= 1.58D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.428D-04 0.834D-03-0.191D-03-0.200D-02-0.143D-01-0.246D-01

Coeff-Com: -0.112D-01 0.118D+00 0.352D+00 0.581D+00

Coeff: -0.428D-04 0.834D-03-0.191D-03-0.200D-02-0.143D-01-0.246D-01

Coeff: -0.112D-01 0.118D+00 0.352D+00 0.581D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=1.36D-07 MaxDP=4.86D-06 DE=-3.84D-09 OVMax= 1.46D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 7.20D-08 CP: 9.98D-01 1.09D+00 7.58D-01 8.12D-01 1.05D+00

CP: 1.06D+00 1.42D+00 1.12D+00 8.69D-01 8.32D-01

E= -1658.67665637281 Delta-E= -0.000000000751 Rises=F Damp=F

DIIS: error= 3.64D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67665637281 IErMin=11 ErrMin= 3.64D-07

ErrMax= 3.64D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.63D-10 BMatP= 2.96D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.132D-04 0.195D-03 0.180D-03 0.217D-03-0.672D-03-0.308D-02

Coeff-Com: -0.182D-01-0.654D-02 0.626D-01 0.216D+00 0.749D+00

Coeff: -0.132D-04 0.195D-03 0.180D-03 0.217D-03-0.672D-03-0.308D-02

Coeff: -0.182D-01-0.654D-02 0.626D-01 0.216D+00 0.749D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=5.27D-08 MaxDP=2.54D-06 DE=-7.51D-10 OVMax= 6.11D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 3.18D-08 CP: 9.98D-01 1.09D+00 7.58D-01 8.12D-01 1.05D+00

CP: 1.06D+00 1.43D+00 1.13D+00 9.32D-01 9.53D-01

CP: 9.41D-01

E= -1658.67665637291 Delta-E= -0.000000000092 Rises=F Damp=F

DIIS: error= 1.47D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.67665637291 IErMin=12 ErrMin= 1.47D-07

ErrMax= 1.47D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.22D-11 BMatP= 1.63D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.226D-05-0.763D-04 0.121D-03 0.503D-03 0.262D-02 0.360D-02

Coeff-Com: -0.636D-02-0.272D-01-0.423D-01-0.170D-01 0.354D+00 0.732D+00

Coeff: 0.226D-05-0.763D-04 0.121D-03 0.503D-03 0.262D-02 0.360D-02

Coeff: -0.636D-02-0.272D-01-0.423D-01-0.170D-01 0.354D+00 0.732D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=2.35D-08 MaxDP=1.24D-06 DE=-9.19D-11 OVMax= 2.20D-06

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.26D-08 CP: 9.98D-01 1.09D+00 7.58D-01 8.12D-01 1.05D+00

CP: 1.06D+00 1.43D+00 1.14D+00 9.42D-01 1.00D+00

CP: 1.15D+00 9.14D-01

E= -1658.67665637293 Delta-E= -0.000000000026 Rises=F Damp=F

DIIS: error= 6.37D-08 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1658.67665637293 IErMin=13 ErrMin= 6.37D-08

ErrMax= 6.37D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.65D-12 BMatP= 4.22D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.323D-05-0.660D-04 0.236D-04 0.181D-03 0.121D-02 0.206D-02

Coeff-Com: 0.704D-03-0.997D-02-0.287D-01-0.467D-01 0.192D-01 0.295D+00

Coeff-Com: 0.767D+00

Coeff: 0.323D-05-0.660D-04 0.236D-04 0.181D-03 0.121D-02 0.206D-02

Coeff: 0.704D-03-0.997D-02-0.287D-01-0.467D-01 0.192D-01 0.295D+00

Coeff: 0.767D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=9.94D-09 MaxDP=3.90D-07 DE=-2.64D-11 OVMax= 1.26D-06

Error on total polarization charges = 0.04147

SCF Done: E(UB3LYP) = -1658.67665637 A.U. after 13 cycles

NFock= 13 Conv=0.99D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655277684143D+03 PE=-6.153850444785D+03 EE= 1.734371218450D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.53

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:37:34 2019, MaxMem= 1342177280 cpu: 318.3

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 333

Leave Link 701 at Sat Aug 17 17:37:35 2019, MaxMem= 1342177280 cpu: 10.3

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:37:35 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:37:38 2019, MaxMem= 1342177280 cpu: 36.4

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.50478585D+00-3.05190379D+00 6.13669598D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.003981822 -0.001885943 0.000035600

2 6 -0.000071080 -0.000891165 0.001550369

3 8 -0.003402076 0.002332245 -0.001433886

4 8 0.000420376 -0.000461104 0.000632895

5 6 -0.000388152 0.000141418 0.000186785

6 16 0.000787229 0.000784265 -0.000830197

7 6 -0.000992031 0.000016603 0.000171399

8 16 0.000797869 -0.000738369 0.000726381

9 16 0.000075756 0.000702403 -0.000361754

10 6 -0.000904167 -0.000650581 -0.000496714

11 6 0.000379339 -0.000200141 -0.000275738

12 6 -0.000363721 0.000189466 -0.000324111

13 6 0.000549258 -0.000520752 -0.000007521

14 1 -0.000451221 0.000861713 -0.000102193

15 1 -0.000762021 -0.000105664 -0.000337044

16 1 0.000654768 -0.000504388 0.000612667

17 1 -0.000509263 0.000071385 0.000333553

18 1 -0.000226496 -0.000410393 -0.000138657

19 1 0.001099834 0.001018127 -0.000505808

20 1 -0.000668597 -0.000063133 0.000690425

21 1 -0.000238249 0.000316159 0.000391225

22 1 0.000436332 -0.000409721 -0.000446039

23 1 0.000020454 0.000109331 -0.000363025

24 1 -0.000123652 0.000079320 0.000358678

25 1 0.000244917 0.000255816 0.000069373

26 1 -0.000099851 -0.000095167 0.000419745

27 1 -0.000247378 0.000058269 -0.000556407

-------------------------------------------------------------------

Cartesian Forces: Max 0.003981822 RMS 0.000854744

Leave Link 716 at Sat Aug 17 17:37:38 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.004492503 RMS 0.000825448

Search for a local minimum.

Step number 18 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .82545D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 4 5 6 8 9

10 11 12 13 14

15 16 17 18

DE= 2.82D-04 DEPred=-6.21D-05 R=-4.54D+00

Trust test=-4.54D+00 RLast= 3.81D-01 DXMaxT set to 8.41D-02

ITU= -1 1 1 -1 1 -1 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Eigenvalues --- 0.00109 0.00238 0.00316 0.00382 0.00464

Eigenvalues --- 0.00531 0.00710 0.01189 0.01700 0.02333

Eigenvalues --- 0.03144 0.03226 0.03537 0.03682 0.04593

Eigenvalues --- 0.04817 0.04837 0.04943 0.05286 0.05447

Eigenvalues --- 0.05466 0.05652 0.05833 0.05929 0.08246

Eigenvalues --- 0.08347 0.08503 0.11321 0.12177 0.12271

Eigenvalues --- 0.14258 0.15510 0.15938 0.16002 0.16038

Eigenvalues --- 0.16069 0.16276 0.16476 0.17231 0.18416

Eigenvalues --- 0.21799 0.21962 0.22124 0.22939 0.23586

Eigenvalues --- 0.24344 0.24664 0.25428 0.25824 0.26689

Eigenvalues --- 0.28225 0.29121 0.29475 0.29778 0.30019

Eigenvalues --- 0.30680 0.32512 0.33517 0.33821 0.33878

Eigenvalues --- 0.33883 0.33949 0.33990 0.34033 0.34052

Eigenvalues --- 0.34121 0.34244 0.34492 0.34553 0.34599

Eigenvalues --- 0.35596 0.41816 0.52672 0.57726 1.51118

En-DIIS/RFO-DIIS IScMMF= 0 using points: 18 17 16 15 14

RFO step: Lambda=-1.58624389D-04.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=T DC= -1.00D-06 SmlDif= 1.00D-05

RMS Error= 0.2264589055D-02 NUsed= 5 EDIIS=F

DidBck=T Rises=T RFO-DIIS coefs: 0.12335 0.28115 0.39406 -0.05522 0.25666

Iteration 1 RMS(Cart)= 0.18133295 RMS(Int)= 0.00725313

Iteration 2 RMS(Cart)= 0.02289438 RMS(Int)= 0.00006983

Iteration 3 RMS(Cart)= 0.00031320 RMS(Int)= 0.00000371

Iteration 4 RMS(Cart)= 0.00000002 RMS(Int)= 0.00000371

ITry= 1 IFail=0 DXMaxC= 6.25D-01 DCOld= 1.00D+10 DXMaxT= 8.41D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83463 0.00027 0.00402 -0.00101 0.00301 2.83764

R2 2.28441 0.00434 0.00225 0.00155 0.00380 2.28821

R3 2.55255 0.00061 0.00063 0.00008 0.00071 2.55326

R4 2.86505 0.00087 0.00134 0.00027 0.00161 2.86666

R5 3.60294 0.00164 -0.00867 0.00265 -0.00603 3.59692

R6 2.05601 0.00084 0.00166 0.00046 0.00212 2.05813

R7 1.83504 0.00082 0.00163 0.00036 0.00199 1.83703

R8 2.05870 0.00050 0.00266 0.00012 0.00277 2.06148

R9 2.06686 0.00056 0.00194 0.00001 0.00195 2.06881

R10 2.05895 0.00034 0.00127 0.00015 0.00142 2.06037

R11 3.31973 -0.00024 0.00157 -0.00092 0.00065 3.32038

R12 3.38555 0.00107 -0.00223 0.00060 -0.00163 3.38392

R13 3.25312 0.00040 0.00126 -0.00019 0.00107 3.25419

R14 3.47149 0.00009 0.00512 -0.00014 0.00498 3.47647

R15 2.87946 0.00055 0.00143 0.00014 0.00157 2.88103

R16 2.06175 0.00106 0.00183 0.00023 0.00206 2.06381

R17 2.05842 0.00050 0.00171 0.00021 0.00192 2.06034

R18 2.89386 0.00000 0.00021 0.00026 0.00047 2.89433

R19 2.07166 0.00013 0.00063 0.00012 0.00076 2.07241

R20 2.06980 0.00058 0.00097 0.00019 0.00116 2.07096

R21 2.88421 0.00053 0.00160 0.00014 0.00174 2.88595

R22 2.07091 0.00035 0.00098 0.00017 0.00116 2.07207

R23 2.07094 0.00033 0.00067 0.00017 0.00084 2.07178

R24 2.06657 0.00034 0.00105 0.00012 0.00117 2.06774

R25 2.06823 0.00040 0.00083 0.00020 0.00103 2.06926

R26 2.06794 0.00041 0.00095 0.00019 0.00114 2.06908

A1 2.17711 0.00003 0.00029 -0.00024 0.00006 2.17716

A2 1.97408 0.00028 0.00081 0.00118 0.00199 1.97607

A3 2.13106 -0.00029 -0.00071 -0.00092 -0.00163 2.12942

A4 2.02651 -0.00087 -0.00454 0.00137 -0.00317 2.02334

A5 1.83832 -0.00163 0.00075 -0.00150 -0.00075 1.83757

A6 1.87679 0.00026 -0.00634 0.00089 -0.00546 1.87133

A7 1.93737 0.00258 0.00972 -0.00058 0.00914 1.94651

A8 1.93537 0.00021 0.00470 -0.00006 0.00465 1.94002

A9 1.83760 -0.00066 -0.00500 -0.00029 -0.00529 1.83231

A10 1.87549 -0.00020 -0.00154 -0.00059 -0.00213 1.87337

A11 1.90461 0.00144 0.00733 -0.00039 0.00693 1.91155

A12 1.93086 -0.00059 -0.00245 0.00016 -0.00229 1.92857

A13 1.95456 -0.00031 -0.00175 -0.00044 -0.00220 1.95236

A14 1.88518 -0.00030 -0.00202 0.00063 -0.00139 1.88378

A15 1.89431 -0.00039 -0.00084 -0.00016 -0.00100 1.89331

A16 1.89272 0.00015 -0.00033 0.00025 -0.00008 1.89264

A17 1.79521 0.00449 -0.00284 0.00070 -0.00215 1.79307

A18 1.96080 0.00062 0.01181 -0.00028 0.01153 1.97233

A19 2.14143 -0.00039 0.00059 -0.00009 0.00050 2.14193

A20 2.15619 0.00035 -0.00349 0.00119 -0.00230 2.15389

A21 1.80043 -0.00092 -0.00764 0.00004 -0.00760 1.79283

A22 1.92414 0.00065 0.00367 0.00090 0.00457 1.92870

A23 1.87190 0.00073 0.00216 0.00043 0.00259 1.87448

A24 1.89647 -0.00092 -0.00049 -0.00074 -0.00122 1.89525

A25 1.94266 -0.00098 -0.00392 -0.00020 -0.00412 1.93854

A26 1.93959 0.00042 -0.00119 -0.00003 -0.00122 1.93837

A27 1.88703 0.00009 -0.00014 -0.00038 -0.00052 1.88650

A28 1.95462 -0.00031 -0.00167 -0.00060 -0.00227 1.95235

A29 1.91842 -0.00026 -0.00034 -0.00001 -0.00035 1.91807

A30 1.91430 0.00051 0.00046 0.00047 0.00093 1.91523

A31 1.90615 0.00035 -0.00033 0.00016 -0.00017 1.90598

A32 1.91071 -0.00034 -0.00024 -0.00026 -0.00050 1.91021

A33 1.85707 0.00007 0.00232 0.00028 0.00260 1.85967

A34 1.96664 0.00009 0.00037 0.00031 0.00068 1.96733

A35 1.90690 -0.00002 -0.00030 -0.00024 -0.00053 1.90637

A36 1.90817 -0.00015 -0.00101 -0.00034 -0.00136 1.90681

A37 1.91413 -0.00012 -0.00151 0.00013 -0.00138 1.91275

A38 1.91140 0.00011 0.00156 -0.00019 0.00137 1.91277

A39 1.85313 0.00009 0.00092 0.00032 0.00124 1.85437

A40 1.94603 -0.00005 -0.00054 -0.00025 -0.00079 1.94524

A41 1.94179 -0.00010 0.00093 -0.00041 0.00052 1.94231

A42 1.94639 -0.00052 -0.00285 0.00008 -0.00277 1.94363

A43 1.87651 0.00009 -0.00041 0.00036 -0.00006 1.87646

A44 1.87651 0.00025 0.00018 0.00033 0.00051 1.87702

A45 1.87296 0.00038 0.00286 -0.00007 0.00279 1.87575

D1 2.72067 -0.00079 -0.07653 0.02313 -0.05341 2.66726

D2 -1.41149 0.00072 -0.06639 0.02212 -0.04427 -1.45577

D3 0.54184 -0.00065 -0.07436 0.02149 -0.05286 0.48898

D4 -0.46700 -0.00029 -0.06537 0.02352 -0.04185 -0.50886

D5 1.68402 0.00122 -0.05523 0.02251 -0.03271 1.65131

D6 -2.64583 -0.00015 -0.06319 0.02188 -0.04131 -2.68713

D7 -3.09344 -0.00031 -0.01108 0.00065 -0.01042 -3.10387

D8 0.00345 0.00018 -0.00023 0.00105 0.00082 0.00427

D9 -3.10156 -0.00028 -0.02046 0.00259 -0.01788 -3.11943

D10 -1.02978 -0.00012 -0.01989 0.00321 -0.01668 -1.04646

D11 1.08389 -0.00056 -0.02320 0.00334 -0.01986 1.06403

D12 1.08318 0.00049 -0.02583 0.00405 -0.02178 1.06139

D13 -3.12823 0.00065 -0.02525 0.00467 -0.02059 3.13437

D14 -1.01456 0.00021 -0.02856 0.00479 -0.02377 -1.03833

D15 -0.95304 -0.00043 -0.02867 0.00481 -0.02386 -0.97690

D16 1.11874 -0.00026 -0.02810 0.00543 -0.02266 1.09607

D17 -3.05078 -0.00070 -0.03141 0.00555 -0.02585 -3.07662

D18 -3.04031 -0.00067 -0.11140 -0.00034 -0.11173 3.13115

D19 -0.83343 -0.00125 -0.11041 -0.00003 -0.11045 -0.94388

D20 1.26196 -0.00001 -0.10255 -0.00059 -0.10314 1.15882

D21 1.77533 0.00158 0.07449 -0.00220 0.07228 1.84761

D22 -1.13640 -0.00109 0.02830 -0.00609 0.02223 -1.11417

D23 2.68601 -0.00186 -0.14581 0.00734 -0.13849 2.54752

D24 -0.68770 0.00073 -0.09868 0.01106 -0.08760 -0.77531

D25 -3.12127 0.00060 0.13369 -0.00120 0.13249 -2.98878

D26 -1.00356 0.00024 0.13243 -0.00065 0.13179 -0.87177

D27 1.03240 0.00027 0.13317 -0.00125 0.13192 1.16432

D28 -3.10048 0.00016 -0.00079 -0.00129 -0.00209 -3.10257

D29 -0.97833 0.00021 -0.00258 -0.00150 -0.00408 -0.98241

D30 1.05764 0.00045 0.00031 -0.00089 -0.00058 1.05706

D31 1.10768 -0.00056 -0.00337 -0.00228 -0.00565 1.10203

D32 -3.05335 -0.00050 -0.00515 -0.00249 -0.00764 -3.06099

D33 -1.01739 -0.00027 -0.00227 -0.00188 -0.00414 -1.02153

D34 -0.99666 -0.00029 0.00026 -0.00164 -0.00138 -0.99805

D35 1.12549 -0.00023 -0.00152 -0.00185 -0.00337 1.12212

D36 -3.12173 0.00000 0.00137 -0.00124 0.00012 -3.12161

D37 3.12985 -0.00005 0.03419 -0.00686 0.02734 -3.12600

D38 -1.02103 -0.00015 0.03230 -0.00664 0.02566 -0.99537

D39 1.00012 -0.00013 0.03268 -0.00658 0.02609 1.02621

D40 1.00066 0.00024 0.03596 -0.00656 0.02940 1.03007

D41 3.13297 0.00014 0.03407 -0.00634 0.02772 -3.12249

D42 -1.12906 0.00016 0.03444 -0.00629 0.02816 -1.10091

D43 -1.02621 0.00015 0.03350 -0.00684 0.02666 -0.99955

D44 1.10609 0.00005 0.03161 -0.00662 0.02498 1.13108

D45 3.12725 0.00006 0.03198 -0.00657 0.02541 -3.13053

D46 3.12268 0.00000 0.02580 -0.00397 0.02183 -3.13868

D47 -1.06573 0.00000 0.02554 -0.00397 0.02158 -1.04415

D48 1.02478 0.00006 0.02788 -0.00428 0.02360 1.04838

D49 0.99446 0.00004 0.02701 -0.00398 0.02303 1.01749

D50 3.08923 0.00005 0.02675 -0.00398 0.02278 3.11201

D51 -1.10345 0.00011 0.02909 -0.00429 0.02480 -1.07864

D52 -1.03260 -0.00006 0.02586 -0.00433 0.02154 -1.01106

D53 1.06217 -0.00006 0.02561 -0.00432 0.02128 1.08346

D54 -3.13051 0.00001 0.02795 -0.00463 0.02331 -3.10720

Item Value Threshold Converged?

Maximum Force 0.004493 0.000450 NO

RMS Force 0.000825 0.000300 NO

Maximum Displacement 0.625352 0.001800 NO

RMS Displacement 0.180591 0.001200 NO

Predicted change in Energy=-2.963781D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:37:38 2019, MaxMem= 1342177280 cpu: 0.6

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.105773 -0.409930 -0.214550

2 6 0 -2.839999 0.052377 0.447969

3 8 0 -4.883783 0.312768 -0.796450

4 8 0 -4.288505 -1.746573 -0.140116

5 6 0 -2.353279 -0.791842 1.610552

6 16 0 -1.545711 0.135003 -0.945209

7 6 0 -0.107764 0.695465 -0.105281

8 16 0 1.108942 -0.595781 0.137409

9 16 0 -0.012001 2.241883 0.646282

10 6 0 2.700645 0.316128 -0.001466

11 6 0 3.872986 -0.657919 -0.035720

12 6 0 5.218627 0.071110 -0.095778

13 6 0 6.406502 -0.886999 -0.152795

14 1 0 -2.994022 1.087099 0.750951

15 1 0 -5.107166 -1.954264 -0.621438

16 1 0 -1.445400 -0.351934 2.025608

17 1 0 -3.106623 -0.821926 2.404331

18 1 0 -2.133074 -1.815055 1.305104

19 1 0 2.657514 0.910934 -0.916381

20 1 0 2.784168 1.000189 0.843407

21 1 0 3.850268 -1.300685 0.852553

22 1 0 3.778108 -1.320792 -0.903246

23 1 0 5.234198 0.728695 -0.973065

24 1 0 5.315070 0.724641 0.779184

25 1 0 7.356256 -0.345063 -0.192141

26 1 0 6.434772 -1.537949 0.727265

27 1 0 6.357206 -1.531218 -1.036754

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.501614 0.000000

3 O 1.210868 2.406956 0.000000

4 O 1.351128 2.383325 2.241878 0.000000

5 C 2.558924 1.516971 3.662960 2.778750 0.000000

6 S 2.717486 1.903406 3.346110 3.422195 2.836040

7 C 4.149447 2.860901 4.840922 4.841834 3.193509

8 S 5.229883 4.013813 6.132725 5.525738 3.767700

9 S 4.952991 3.582016 5.434816 5.900398 3.951567

10 C 6.848350 5.565096 7.625980 7.288496 5.419257

11 C 7.984615 6.767765 8.843187 8.234440 6.441624

12 C 9.337556 8.076972 10.129563 9.679437 7.809610

13 C 10.523276 9.313492 11.372083 10.729502 8.936007

14 H 2.099829 1.089115 2.562272 3.240276 2.163304

15 H 1.885023 3.210963 2.284725 0.972117 3.730536

16 H 3.478398 2.144136 4.497591 3.836486 1.090887

17 H 2.833121 2.159362 3.832862 2.953985 1.094768

18 H 2.859242 2.172954 4.063320 2.596004 1.090300

19 H 6.926710 5.728981 7.565934 7.477440 5.864545

20 H 7.111892 5.717166 7.871414 7.650799 5.494839

21 H 8.076555 6.837700 9.033609 8.211201 6.270365

22 H 7.966150 6.892802 8.815230 8.113809 6.647772

23 H 9.439644 8.226142 10.128067 9.874342 8.158242

24 H 9.540810 8.189433 10.328063 9.958949 7.860946

25 H 11.462235 10.224056 12.272591 11.728913 9.885565

26 H 10.642487 9.414272 11.569639 10.760322 8.863786

27 H 10.554963 9.449908 11.393764 10.685574 9.133863

6 7 8 9 10

6 S 0.000000

7 C 1.757068 0.000000

8 S 2.958596 1.790695 0.000000

9 S 3.053532 1.722041 3.093186 0.000000

10 C 4.353734 2.835813 1.839669 3.389182 0.000000

11 C 5.551412 4.205099 2.770157 4.895620 1.524573

12 C 6.817763 5.362868 4.169968 5.711600 2.531632

13 C 8.056681 6.703888 5.313490 7.185096 3.899204

14 H 2.425088 3.035950 4.476922 3.199520 5.795667

15 H 4.141717 5.681681 6.407911 6.721270 8.154812

16 H 3.012129 2.725252 3.185815 3.268801 4.663156

17 H 3.817273 4.194494 4.791771 4.696206 6.388066

18 H 3.035067 3.520479 3.655244 4.625121 5.441866

19 H 4.274343 2.889823 2.403900 3.367440 1.092119

20 H 4.763985 3.058781 2.419077 3.065816 1.090287

21 H 5.865981 4.535204 2.919450 5.244945 2.159876

22 H 5.519434 4.449948 2.955173 5.427578 2.157230

23 H 6.805911 5.412090 4.472709 5.695140 2.744651

24 H 7.098699 5.494567 4.454986 5.540521 2.758898

25 H 8.946653 7.536700 6.261022 7.854072 4.706192

26 H 8.323704 6.963192 5.440595 7.473591 4.232299

27 H 8.077176 6.900840 5.458752 7.591817 4.225511

11 12 13 14 15

11 C 0.000000

12 C 1.531614 0.000000

13 C 2.546545 1.527178 0.000000

14 H 7.128796 8.318460 9.647988 0.000000

15 H 9.092123 10.535676 11.572520 3.949522 0.000000

16 H 5.712086 7.006319 8.166033 2.468562 4.794042

17 H 7.395653 8.738298 9.851024 2.527988 3.799952

18 H 6.261751 7.718005 8.712699 3.077469 3.546289

19 H 2.171229 2.817445 4.227356 5.894988 8.281703

20 H 2.169725 2.769810 4.204188 5.779583 8.552644

21 H 1.096674 2.157211 2.777804 7.249561 9.101397

22 H 1.095903 2.159744 2.767636 7.375367 8.912283

23 H 2.157362 1.096491 2.158149 8.414528 10.689514

24 H 2.157579 1.096340 2.158053 8.317042 10.851787

25 H 3.500788 2.179895 1.094201 10.491366 12.574208

26 H 2.814133 2.178412 1.095007 9.787420 11.627925

27 H 2.817103 2.179278 1.094911 9.874053 11.479689

16 17 18 19 20

16 H 0.000000

17 H 1.767480 0.000000

18 H 1.769956 1.772682 0.000000

19 H 5.204233 6.874242 5.942705 0.000000

20 H 4.595115 6.360661 5.684895 1.766597 0.000000

21 H 5.506385 7.143917 6.022437 3.072954 2.535876

22 H 6.066457 7.654309 6.329547 2.497299 3.070124

23 H 7.401137 9.131294 8.120185 2.583742 3.062013

24 H 6.958200 8.715383 7.886793 3.157887 2.546668

25 H 9.076762 10.790779 9.718539 4.917340 4.877094

26 H 8.073997 9.714085 8.591779 4.792314 4.447756

27 H 8.464598 10.094960 8.811907 4.434672 4.765461

21 22 23 24 25

21 H 0.000000

22 H 1.757396 0.000000

23 H 3.060478 2.515049 0.000000

24 H 2.500595 3.062127 1.754118 0.000000

25 H 3.781079 3.776356 2.503184 2.500836 0.000000

26 H 2.598394 3.124674 3.077365 2.525023 1.765622

27 H 3.147596 2.591110 2.524363 3.077755 1.765909

26 27

26 H 0.000000

27 H 1.765736 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 4.12D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.118651 -0.421035 -0.162367

2 6 0 -2.845852 0.112239 0.429615

3 8 0 -4.897745 0.228977 -0.823198

4 8 0 -4.306855 -1.737429 0.076865

5 6 0 -2.354215 -0.585528 1.683656

6 16 0 -1.561725 0.016249 -0.972083

7 6 0 -0.114980 0.667778 -0.217279

8 16 0 1.097672 -0.590479 0.173683

9 16 0 -0.006578 2.294206 0.338064

10 6 0 2.692389 0.288870 -0.087098

11 6 0 3.860026 -0.688342 -0.009614

12 6 0 5.208457 0.020517 -0.168023

13 6 0 6.391529 -0.943757 -0.115193

14 1 0 -2.992913 1.177143 0.604330

15 1 0 -5.130044 -1.998194 -0.369645

16 1 0 -1.441260 -0.102921 2.035276

17 1 0 -3.101692 -0.513887 2.480312

18 1 0 -2.140940 -1.639670 1.504623

19 1 0 2.645061 0.767112 -1.067796

20 1 0 2.785358 1.070992 0.666804

21 1 0 3.841089 -1.217095 0.950987

22 1 0 3.755628 -1.452156 -0.788519

23 1 0 5.220396 0.565363 -1.119491

24 1 0 5.314434 0.775963 0.619398

25 1 0 7.343398 -0.415890 -0.227341

26 1 0 6.423479 -1.481914 0.837910

27 1 0 6.332671 -1.691320 -0.913012

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3291400 0.1919033 0.1799616

Leave Link 202 at Sat Aug 17 17:37:38 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1101.4294329812 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0549142905 Hartrees.

Nuclear repulsion after empirical dispersion term = 1101.3745186907 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2318

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.96D-09

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 101

GePol: Fraction of low-weight points (<1% of avg) = 4.36%

GePol: Cavity surface area = 309.454 Ang\*\*2

GePol: Cavity volume = 320.168 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0058025813 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1101.3687161095 Hartrees.

Leave Link 301 at Sat Aug 17 17:37:38 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:37:39 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:37:39 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999749 0.022062 0.003802 0.000934 Ang= 2.57 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.62983545846

Leave Link 401 at Sat Aug 17 17:37:39 2019, MaxMem= 1342177280 cpu: 7.5

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16119372.

Iteration 1 A\*A^-1 deviation from unit magnitude is 3.89D-15 for 2289.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.52D-15 for 2286 48.

Iteration 1 A^-1\*A deviation from unit magnitude is 4.22D-15 for 2305.

Iteration 1 A^-1\*A deviation from orthogonality is 4.33D-13 for 918 911.

E= -1658.63104008666

DIIS: error= 7.75D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.63104008666 IErMin= 1 ErrMin= 7.75D-03

ErrMax= 7.75D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.75D-02 BMatP= 9.75D-02

IDIUse=3 WtCom= 9.23D-01 WtEn= 7.75D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.429 Goal= None Shift= 0.000

Gap= 0.483 Goal= None Shift= 0.000

GapD= 0.429 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=8.18D-04 MaxDP=2.82D-02 OVMax= 5.04D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 8.17D-04 CP: 9.97D-01

E= -1658.67631735758 Delta-E= -0.045277270924 Rises=F Damp=F

DIIS: error= 8.29D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67631735758 IErMin= 2 ErrMin= 8.29D-04

ErrMax= 8.29D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.70D-03 BMatP= 9.75D-02

IDIUse=3 WtCom= 9.92D-01 WtEn= 8.29D-03

Coeff-Com: -0.614D-01 0.106D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.609D-01 0.106D+01

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=1.33D-04 MaxDP=4.33D-03 DE=-4.53D-02 OVMax= 7.93D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.28D-04 CP: 9.97D-01 1.04D+00

E= -1658.67677055671 Delta-E= -0.000453199132 Rises=F Damp=F

DIIS: error= 5.44D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67677055671 IErMin= 3 ErrMin= 5.44D-04

ErrMax= 5.44D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.55D-04 BMatP= 1.70D-03

IDIUse=3 WtCom= 9.95D-01 WtEn= 5.44D-03

Coeff-Com: -0.316D-01 0.442D+00 0.590D+00

Coeff-En: 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.314D-01 0.439D+00 0.592D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=8.26D-05 MaxDP=2.99D-03 DE=-4.53D-04 OVMax= 9.25D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 6.26D-05 CP: 9.97D-01 1.08D+00 6.45D-01

E= -1658.67688446527 Delta-E= -0.000113908553 Rises=F Damp=F

DIIS: error= 4.44D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67688446527 IErMin= 4 ErrMin= 4.44D-04

ErrMax= 4.44D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.53D-04 BMatP= 7.55D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 4.44D-03

Coeff-Com: -0.132D-01 0.170D+00 0.408D+00 0.435D+00

Coeff-En: 0.000D+00 0.000D+00 0.317D+00 0.683D+00

Coeff: -0.131D-01 0.170D+00 0.407D+00 0.436D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.34D-05 MaxDP=1.60D-03 DE=-1.14D-04 OVMax= 3.32D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.09D-05 CP: 9.97D-01 1.09D+00 7.27D-01 6.29D-01

E= -1658.67697116814 Delta-E= -0.000086702876 Rises=F Damp=F

DIIS: error= 5.01D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67697116814 IErMin= 5 ErrMin= 5.01D-05

ErrMax= 5.01D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.98D-06 BMatP= 3.53D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.169D-02 0.141D-01 0.104D+00 0.171D+00 0.712D+00

Coeff: -0.169D-02 0.141D-01 0.104D+00 0.171D+00 0.712D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=8.15D-06 MaxDP=2.84D-04 DE=-8.67D-05 OVMax= 7.98D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 5.52D-06 CP: 9.97D-01 1.09D+00 7.53D-01 7.06D-01 9.49D-01

E= -1658.67697331739 Delta-E= -0.000002149241 Rises=F Damp=F

DIIS: error= 4.87D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67697331739 IErMin= 6 ErrMin= 4.87D-05

ErrMax= 4.87D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.21D-06 BMatP= 7.98D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.104D-02-0.185D-01 0.870D-03 0.310D-01 0.393D+00 0.593D+00

Coeff: 0.104D-02-0.185D-01 0.870D-03 0.310D-01 0.393D+00 0.593D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.93D-06 MaxDP=1.74D-04 DE=-2.15D-06 OVMax= 4.58D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.70D-06 CP: 9.97D-01 1.09D+00 7.64D-01 7.32D-01 1.02D+00

CP: 8.30D-01

E= -1658.67697398749 Delta-E= -0.000000670109 Rises=F Damp=F

DIIS: error= 1.31D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67697398749 IErMin= 7 ErrMin= 1.31D-05

ErrMax= 1.31D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.78D-07 BMatP= 2.21D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.590D-03-0.847D-02-0.135D-01-0.139D-01 0.382D-01 0.221D+00

Coeff-Com: 0.776D+00

Coeff: 0.590D-03-0.847D-02-0.135D-01-0.139D-01 0.382D-01 0.221D+00

Coeff: 0.776D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.82D-06 MaxDP=7.51D-05 DE=-6.70D-07 OVMax= 2.42D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 9.29D-07 CP: 9.97D-01 1.09D+00 7.67D-01 7.42D-01 1.07D+00

CP: 1.00D+00 1.10D+00

E= -1658.67697406096 Delta-E= -0.000000073469 Rises=F Damp=F

DIIS: error= 6.52D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67697406096 IErMin= 8 ErrMin= 6.52D-06

ErrMax= 6.52D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.19D-08 BMatP= 1.78D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.160D-03-0.150D-02-0.780D-02-0.139D-01-0.470D-01 0.292D-01

Coeff-Com: 0.455D+00 0.585D+00

Coeff: 0.160D-03-0.150D-02-0.780D-02-0.139D-01-0.470D-01 0.292D-01

Coeff: 0.455D+00 0.585D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=7.84D-07 MaxDP=3.20D-05 DE=-7.35D-08 OVMax= 1.02D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 3.73D-07 CP: 9.97D-01 1.09D+00 7.67D-01 7.48D-01 1.08D+00

CP: 1.05D+00 1.25D+00 9.06D-01

E= -1658.67697407991 Delta-E= -0.000000018947 Rises=F Damp=F

DIIS: error= 4.78D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67697407991 IErMin= 9 ErrMin= 4.78D-06

ErrMax= 4.78D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.50D-08 BMatP= 7.19D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.421D-04 0.114D-02-0.186D-02-0.575D-02-0.395D-01-0.355D-01

Coeff-Com: 0.948D-01 0.354D+00 0.633D+00

Coeff: -0.421D-04 0.114D-02-0.186D-02-0.575D-02-0.395D-01-0.355D-01

Coeff: 0.948D-01 0.354D+00 0.633D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.47D-07 MaxDP=1.29D-05 DE=-1.89D-08 OVMax= 5.01D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.53D-07 CP: 9.97D-01 1.09D+00 7.68D-01 7.50D-01 1.08D+00

CP: 1.07D+00 1.32D+00 1.02D+00 8.12D-01

E= -1658.67697408363 Delta-E= -0.000000003719 Rises=F Damp=F

DIIS: error= 2.43D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67697408363 IErMin=10 ErrMin= 2.43D-06

ErrMax= 2.43D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.96D-09 BMatP= 1.50D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.456D-04 0.872D-03-0.169D-03-0.172D-02-0.173D-01-0.246D-01

Coeff-Com: -0.462D-02 0.135D+00 0.390D+00 0.522D+00

Coeff: -0.456D-04 0.872D-03-0.169D-03-0.172D-02-0.173D-01-0.246D-01

Coeff: -0.462D-02 0.135D+00 0.390D+00 0.522D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.11D-07 MaxDP=3.63D-06 DE=-3.72D-09 OVMax= 1.13D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 6.41D-08 CP: 9.97D-01 1.09D+00 7.68D-01 7.51D-01 1.08D+00

CP: 1.08D+00 1.34D+00 1.05D+00 9.22D-01 8.52D-01

E= -1658.67697408434 Delta-E= -0.000000000709 Rises=F Damp=F

DIIS: error= 5.93D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67697408434 IErMin=11 ErrMin= 5.93D-07

ErrMax= 5.93D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.14D-10 BMatP= 2.96D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.113D-04 0.160D-03 0.212D-03 0.231D-03-0.282D-03-0.374D-02

Coeff-Com: -0.184D-01-0.612D-02 0.568D-01 0.222D+00 0.749D+00

Coeff: -0.113D-04 0.160D-03 0.212D-03 0.231D-03-0.282D-03-0.374D-02

Coeff: -0.184D-01-0.612D-02 0.568D-01 0.222D+00 0.749D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.86D-08 MaxDP=2.19D-06 DE=-7.09D-10 OVMax= 4.89D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 2.60D-08 CP: 9.97D-01 1.09D+00 7.68D-01 7.51D-01 1.08D+00

CP: 1.08D+00 1.34D+00 1.08D+00 9.76D-01 9.75D-01

CP: 1.07D+00

E= -1658.67697408443 Delta-E= -0.000000000095 Rises=F Damp=F

DIIS: error= 2.00D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.67697408443 IErMin=12 ErrMin= 2.00D-07

ErrMax= 2.00D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.63D-11 BMatP= 2.14D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.278D-05-0.839D-04 0.135D-03 0.454D-03 0.316D-02 0.297D-02

Coeff-Com: -0.777D-02-0.286D-01-0.460D-01 0.701D-02 0.355D+00 0.714D+00

Coeff: 0.278D-05-0.839D-04 0.135D-03 0.454D-03 0.316D-02 0.297D-02

Coeff: -0.777D-02-0.286D-01-0.460D-01 0.701D-02 0.355D+00 0.714D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.21D-08 MaxDP=7.12D-07 DE=-9.55D-11 OVMax= 2.68D-06

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.09D-08 CP: 9.97D-01 1.09D+00 7.68D-01 7.51D-01 1.08D+00

CP: 1.08D+00 1.34D+00 1.08D+00 9.98D-01 1.04D+00

CP: 1.23D+00 1.09D+00

E= -1658.67697408440 Delta-E= 0.000000000036 Rises=F Damp=F

DIIS: error= 8.20D-08 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=12 EnMin= -1658.67697408443 IErMin=13 ErrMin= 8.20D-08

ErrMax= 8.20D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.02D-12 BMatP= 4.63D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.315D-05-0.628D-04 0.199D-04 0.147D-03 0.128D-02 0.191D-02

Coeff-Com: 0.168D-03-0.102D-01-0.299D-01-0.382D-01 0.511D-02 0.273D+00

Coeff-Com: 0.797D+00

Coeff: 0.315D-05-0.628D-04 0.199D-04 0.147D-03 0.128D-02 0.191D-02

Coeff: 0.168D-03-0.102D-01-0.299D-01-0.382D-01 0.511D-02 0.273D+00

Coeff: 0.797D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=9.31D-09 MaxDP=3.24D-07 DE= 3.59D-11 OVMax= 1.05D-06

Error on total polarization charges = 0.04169

SCF Done: E(UB3LYP) = -1658.67697408 A.U. after 13 cycles

NFock= 13 Conv=0.93D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655235536066D+03 PE=-6.145500774864D+03 EE= 1.730219548605D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.64

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:38:06 2019, MaxMem= 1342177280 cpu: 313.7

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 338

Leave Link 701 at Sat Aug 17 17:38:07 2019, MaxMem= 1342177280 cpu: 10.2

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:38:07 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:38:10 2019, MaxMem= 1342177280 cpu: 36.1

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.35816336D+00-2.91084667D+00 5.87462677D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000269247 -0.000145558 -0.000080422

2 6 -0.000353573 -0.000245966 0.000324102

3 8 -0.000193078 0.000144401 -0.000065476

4 8 0.000087559 -0.000018673 0.000059382

5 6 0.000139138 -0.000010416 -0.000041337

6 16 0.000134435 0.000285888 -0.000131149

7 6 -0.000133906 0.000096661 -0.000141309

8 16 0.000370169 -0.000038697 -0.000004170

9 16 -0.000064562 -0.000095323 0.000224854

10 6 -0.000217193 0.000007247 -0.000025492

11 6 -0.000032282 -0.000082682 0.000022492

12 6 -0.000067795 0.000068151 -0.000074545

13 6 0.000038507 -0.000104809 0.000010584

14 1 0.000060614 0.000030930 -0.000070882

15 1 -0.000012768 0.000089766 0.000002214

16 1 0.000070683 -0.000044805 0.000058489

17 1 0.000013357 0.000011068 -0.000005965

18 1 -0.000060125 -0.000011515 -0.000030938

19 1 0.000106853 0.000119156 -0.000018537

20 1 -0.000121582 -0.000102195 0.000059090

21 1 -0.000048864 0.000046310 0.000015857

22 1 0.000033473 -0.000028074 -0.000027802

23 1 0.000000924 0.000007583 0.000016695

24 1 0.000034338 -0.000030137 0.000026670

25 1 -0.000012132 0.000007625 -0.000025962

26 1 0.000004417 -0.000005307 -0.000033215

27 1 -0.000045855 0.000049372 -0.000043227

-------------------------------------------------------------------

Cartesian Forces: Max 0.000370169 RMS 0.000113483

Leave Link 716 at Sat Aug 17 17:38:11 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000627817 RMS 0.000133219

Search for a local minimum.

Step number 19 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .13322D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 19

DE= -3.18D-04 DEPred=-2.96D-04 R= 1.07D+00

TightC=F SS= 1.41D+00 RLast= 3.85D-01 DXNew= 1.4142D-01 1.1564D+00

Trust test= 1.07D+00 RLast= 3.85D-01 DXMaxT set to 1.41D-01

ITU= 1 -1 1 1 -1 1 -1 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Eigenvalues --- 0.00000 0.00023 0.00305 0.00384 0.00432

Eigenvalues --- 0.00497 0.00896 0.00950 0.02036 0.02362

Eigenvalues --- 0.02721 0.03461 0.03581 0.04356 0.04586

Eigenvalues --- 0.04836 0.04863 0.05167 0.05343 0.05473

Eigenvalues --- 0.05509 0.05706 0.05745 0.05879 0.08219

Eigenvalues --- 0.08355 0.08525 0.11372 0.12076 0.12260

Eigenvalues --- 0.14555 0.15606 0.15774 0.16006 0.16026

Eigenvalues --- 0.16068 0.16375 0.16412 0.17303 0.18483

Eigenvalues --- 0.21461 0.21892 0.22219 0.22859 0.23300

Eigenvalues --- 0.24183 0.24686 0.25658 0.26136 0.26741

Eigenvalues --- 0.28494 0.29112 0.29345 0.29503 0.29835

Eigenvalues --- 0.30543 0.31513 0.32843 0.33841 0.33878

Eigenvalues --- 0.33882 0.33957 0.33986 0.34034 0.34049

Eigenvalues --- 0.34132 0.34415 0.34475 0.34566 0.34616

Eigenvalues --- 0.34865 0.41600 0.52560 0.59304 1.32540

Eigenvalue 1 is 5.81D-07 Eigenvector:

D4 D1 D5 D2 D6

1 -0.36619 -0.36415 -0.34932 -0.34728 -0.34198

D3 D24 D23 D43 D37

1 -0.33995 -0.17358 -0.12841 0.10176 0.10167

En-DIIS/RFO-DIIS IScMMF= 0 using points: 19 18 17 16 15

RFO step: Lambda=-1.37807482D-05.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 3.07D-05 SmlDif= 1.00D-05

RMS Error= 0.2121728155D-02 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.11659 0.09838 1.59183 -0.54129 -1.26550

Iteration 1 RMS(Cart)= 0.16371964 RMS(Int)= 0.01241984

Iteration 2 RMS(Cart)= 0.04710529 RMS(Int)= 0.00051526

Iteration 3 RMS(Cart)= 0.00106451 RMS(Int)= 0.00006054

Iteration 4 RMS(Cart)= 0.00000050 RMS(Int)= 0.00006054

ITry= 1 IFail=0 DXMaxC= 7.43D-01 DCOld= 1.00D+10 DXMaxT= 1.41D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83764 -0.00010 -0.00634 -0.00390 -0.01024 2.82740

R2 2.28821 0.00023 -0.00396 0.00509 0.00113 2.28933

R3 2.55326 -0.00003 -0.00230 0.00053 -0.00177 2.55149

R4 2.86666 0.00001 -0.00031 0.00184 0.00153 2.86819

R5 3.59692 0.00012 0.00470 0.01481 0.01952 3.61643

R6 2.05813 0.00000 -0.00255 0.00132 -0.00123 2.05690

R7 1.83703 -0.00002 -0.00237 0.00097 -0.00141 1.83563

R8 2.06148 0.00008 -0.00288 -0.00010 -0.00298 2.05850

R9 2.06881 -0.00001 -0.00213 0.00007 -0.00206 2.06675

R10 2.06037 -0.00003 -0.00195 0.00009 -0.00186 2.05851

R11 3.32038 -0.00018 0.00028 -0.00187 -0.00159 3.31879

R12 3.38392 0.00013 0.00388 0.00322 0.00709 3.39102

R13 3.25419 -0.00001 -0.00302 -0.00138 -0.00439 3.24979

R14 3.47647 -0.00033 -0.00683 -0.00400 -0.01082 3.46565

R15 2.88103 0.00000 -0.00145 0.00091 -0.00055 2.88048

R16 2.06381 0.00009 -0.00222 0.00208 -0.00014 2.06366

R17 2.06034 -0.00004 -0.00244 0.00041 -0.00203 2.05831

R18 2.89433 -0.00005 -0.00111 0.00013 -0.00098 2.89335

R19 2.07241 0.00000 -0.00145 0.00040 -0.00104 2.07137

R20 2.07096 0.00003 -0.00154 0.00111 -0.00043 2.07053

R21 2.88595 0.00004 -0.00133 0.00110 -0.00023 2.88572

R22 2.07207 -0.00001 -0.00178 0.00043 -0.00135 2.07072

R23 2.07178 0.00000 -0.00133 0.00065 -0.00068 2.07111

R24 2.06774 -0.00001 -0.00178 0.00029 -0.00149 2.06625

R25 2.06926 0.00000 -0.00160 0.00082 -0.00078 2.06849

R26 2.06908 -0.00001 -0.00160 0.00059 -0.00101 2.06807

A1 2.17716 0.00014 0.00343 0.00045 0.00361 2.18077

A2 1.97607 -0.00019 -0.00343 0.00286 -0.00084 1.97523

A3 2.12942 0.00005 -0.00009 -0.00190 -0.00227 2.12715

A4 2.02334 -0.00001 -0.00111 -0.00142 -0.00254 2.02080

A5 1.83757 0.00004 0.00538 -0.00582 -0.00045 1.83711

A6 1.87133 0.00008 0.00747 0.00316 0.01064 1.88197

A7 1.94651 -0.00002 -0.00796 0.00400 -0.00398 1.94253

A8 1.94002 -0.00001 -0.00180 0.00049 -0.00133 1.93869

A9 1.83231 -0.00009 -0.00128 -0.00062 -0.00191 1.83039

A10 1.87337 -0.00010 0.00134 0.00018 0.00152 1.87489

A11 1.91155 0.00007 -0.00368 0.00320 -0.00048 1.91107

A12 1.92857 -0.00006 0.00267 -0.00313 -0.00046 1.92811

A13 1.95236 -0.00002 -0.00086 -0.00185 -0.00272 1.94964

A14 1.88378 -0.00002 0.00103 0.00133 0.00236 1.88614

A15 1.89331 0.00000 0.00034 0.00102 0.00136 1.89466

A16 1.89264 0.00003 0.00058 -0.00042 0.00015 1.89280

A17 1.79307 -0.00063 0.00136 0.00778 0.00914 1.80221

A18 1.97233 -0.00027 -0.01475 -0.00219 -0.01719 1.95514

A19 2.14193 0.00012 0.00217 -0.00027 0.00165 2.14358

A20 2.15389 0.00006 0.00588 0.00223 0.00784 2.16173

A21 1.79283 0.00046 0.00990 0.00542 0.01531 1.80814

A22 1.92870 -0.00050 -0.00662 -0.00486 -0.01149 1.91721

A23 1.87448 0.00024 0.00079 0.00844 0.00925 1.88374

A24 1.89525 0.00008 0.00086 -0.00529 -0.00445 1.89079

A25 1.93854 0.00013 0.00362 0.00051 0.00414 1.94268

A26 1.93837 0.00011 0.00130 0.00120 0.00246 1.94083

A27 1.88650 -0.00004 0.00012 0.00020 0.00032 1.88683

A28 1.95235 0.00020 0.00359 0.00226 0.00584 1.95820

A29 1.91807 -0.00014 -0.00107 -0.00329 -0.00438 1.91369

A30 1.91523 0.00001 -0.00046 0.00212 0.00168 1.91690

A31 1.90598 0.00001 0.00117 0.00246 0.00363 1.90961

A32 1.91021 -0.00012 -0.00148 -0.00463 -0.00611 1.90409

A33 1.85967 0.00004 -0.00202 0.00100 -0.00101 1.85865

A34 1.96733 -0.00015 -0.00151 -0.00200 -0.00351 1.96382

A35 1.90637 0.00003 -0.00037 -0.00188 -0.00226 1.90411

A36 1.90681 0.00008 0.00226 0.00207 0.00433 1.91114

A37 1.91275 0.00005 0.00089 -0.00071 0.00018 1.91293

A38 1.91277 0.00002 -0.00093 0.00047 -0.00046 1.91232

A39 1.85437 -0.00002 -0.00026 0.00231 0.00205 1.85642

A40 1.94524 0.00000 0.00057 -0.00003 0.00054 1.94579

A41 1.94231 0.00001 -0.00095 -0.00116 -0.00211 1.94021

A42 1.94363 -0.00006 0.00184 -0.00213 -0.00029 1.94334

A43 1.87646 0.00000 0.00032 0.00118 0.00150 1.87796

A44 1.87702 0.00003 0.00024 0.00162 0.00186 1.87888

A45 1.87575 0.00003 -0.00214 0.00074 -0.00140 1.87435

D1 2.66726 -0.00001 0.00834 0.02776 0.03608 2.70333

D2 -1.45577 0.00000 0.00147 0.02752 0.02896 -1.42680

D3 0.48898 -0.00005 0.00550 0.02557 0.03105 0.52003

D4 -0.50886 0.00006 0.00559 0.07333 0.07894 -0.42992

D5 1.65131 0.00007 -0.00128 0.07309 0.07183 1.72313

D6 -2.68713 0.00002 0.00275 0.07114 0.07391 -2.61323

D7 -3.10387 -0.00007 0.00068 -0.02664 -0.02590 -3.12977

D8 0.00427 0.00000 -0.00190 0.01756 0.01560 0.01988

D9 -3.11943 -0.00002 0.02287 -0.00351 0.01937 -3.10006

D10 -1.04646 -0.00004 0.02348 -0.00180 0.02169 -1.02477

D11 1.06403 -0.00006 0.02548 -0.00575 0.01974 1.08376

D12 1.06139 -0.00006 0.02284 0.00215 0.02499 1.08638

D13 3.13437 -0.00008 0.02345 0.00386 0.02731 -3.12151

D14 -1.03833 -0.00010 0.02545 -0.00009 0.02536 -1.01298

D15 -0.97690 0.00007 0.03064 0.00008 0.03071 -0.94619

D16 1.09607 0.00005 0.03125 0.00179 0.03303 1.12910

D17 -3.07662 0.00003 0.03325 -0.00216 0.03108 -3.04555

D18 3.13115 0.00029 0.08030 0.02025 0.10054 -3.05149

D19 -0.94388 0.00030 0.07761 0.01697 0.09458 -0.84931

D20 1.15882 0.00022 0.07031 0.01935 0.08967 1.24849

D21 1.84761 -0.00030 -0.04113 -0.00117 -0.04221 1.80540

D22 -1.11417 0.00025 -0.00218 -0.00001 -0.00227 -1.11644

D23 2.54752 0.00028 0.09996 0.01668 0.11667 2.66419

D24 -0.77531 -0.00028 0.06028 0.01521 0.07546 -0.69985

D25 -2.98878 -0.00017 -0.17184 -0.08459 -0.25640 3.03801

D26 -0.87177 -0.00017 -0.17085 -0.08156 -0.25242 -1.12419

D27 1.16432 -0.00005 -0.16984 -0.07957 -0.24944 0.91489

D28 -3.10257 0.00001 -0.02173 -0.03983 -0.06155 3.11906

D29 -0.98241 0.00006 -0.01858 -0.03747 -0.05607 -1.03847

D30 1.05706 0.00003 -0.02193 -0.03693 -0.05887 0.99818

D31 1.10203 -0.00004 -0.02074 -0.04754 -0.06827 1.03376

D32 -3.06099 0.00000 -0.01760 -0.04519 -0.06278 -3.12378

D33 -1.02153 -0.00003 -0.02095 -0.04465 -0.06559 -1.08712

D34 -0.99805 -0.00014 -0.02421 -0.04895 -0.07314 -1.07119

D35 1.12212 -0.00010 -0.02106 -0.04659 -0.06766 1.05446

D36 -3.12161 -0.00013 -0.02441 -0.04605 -0.07046 3.09111

D37 -3.12600 -0.00004 -0.03511 -0.00508 -0.04019 3.11700

D38 -0.99537 -0.00006 -0.03526 -0.00867 -0.04391 -1.03929

D39 1.02621 -0.00002 -0.03452 -0.00580 -0.04031 0.98590

D40 1.03007 0.00000 -0.03693 -0.00411 -0.04105 0.98902

D41 -3.12249 -0.00002 -0.03707 -0.00770 -0.04477 3.11592

D42 -1.10091 0.00003 -0.03633 -0.00483 -0.04117 -1.14208

D43 -0.99955 0.00002 -0.03433 -0.00410 -0.03843 -1.03798

D44 1.13108 0.00000 -0.03447 -0.00768 -0.04216 1.08892

D45 -3.13053 0.00005 -0.03374 -0.00482 -0.03856 3.11410

D46 -3.13868 -0.00003 -0.03417 -0.03035 -0.06452 3.07999

D47 -1.04415 -0.00002 -0.03402 -0.02965 -0.06368 -1.10783

D48 1.04838 -0.00002 -0.03613 -0.03094 -0.06706 0.98132

D49 1.01749 0.00000 -0.03331 -0.02608 -0.05939 0.95810

D50 3.11201 0.00001 -0.03315 -0.02539 -0.05854 3.05347

D51 -1.07864 0.00001 -0.03526 -0.02667 -0.06193 -1.14057

D52 -1.01106 -0.00002 -0.03297 -0.02873 -0.06170 -1.07276

D53 1.08346 -0.00001 -0.03282 -0.02803 -0.06085 1.02260

D54 -3.10720 -0.00001 -0.03492 -0.02932 -0.06424 3.11175

Item Value Threshold Converged?

Maximum Force 0.000628 0.000450 NO

RMS Force 0.000133 0.000300 YES

Maximum Displacement 0.742675 0.001800 NO

RMS Displacement 0.200460 0.001200 NO

Predicted change in Energy=-1.545046D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:38:11 2019, MaxMem= 1342177280 cpu: 0.6

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.091979 -0.434141 -0.106621

2 6 0 -2.822583 0.069701 0.504423

3 8 0 -4.964841 0.266427 -0.570258

4 8 0 -4.192261 -1.780489 -0.089073

5 6 0 -2.166737 -0.850774 1.517463

6 16 0 -1.657316 0.420710 -0.972509

7 6 0 -0.144278 0.859622 -0.196359

8 16 0 1.054142 -0.474666 -0.255597

9 16 0 0.025186 2.256481 0.792322

10 6 0 2.668828 0.393553 -0.207356

11 6 0 3.800025 -0.622804 -0.103181

12 6 0 5.177948 0.044595 -0.090842

13 6 0 6.315428 -0.964753 0.047926

14 1 0 -3.026399 1.047086 0.937937

15 1 0 -5.034755 -2.014931 -0.511927

16 1 0 -1.279479 -0.368542 1.925904

17 1 0 -2.851126 -1.058558 2.344848

18 1 0 -1.870803 -1.798188 1.068646

19 1 0 2.755850 0.992362 -1.116428

20 1 0 2.668208 1.071050 0.645511

21 1 0 3.676260 -1.219899 0.807665

22 1 0 3.748671 -1.323584 -0.943882

23 1 0 5.306559 0.618620 -1.015334

24 1 0 5.226756 0.767940 0.731088

25 1 0 7.292518 -0.477126 -0.007432

26 1 0 6.262047 -1.491105 1.006177

27 1 0 6.276292 -1.720227 -0.742887

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.496195 0.000000

3 O 1.211464 2.404769 0.000000

4 O 1.350191 2.377279 2.240153 0.000000

5 C 2.552996 1.517781 3.665529 2.747375 0.000000

6 S 2.721786 1.913735 3.335466 3.471553 2.841856

7 C 4.155264 2.878956 4.871295 4.834031 3.154835

8 S 5.148437 3.987852 6.072594 5.409034 3.695844

9 S 4.999859 3.602038 5.542320 5.904307 3.871097

10 C 6.812028 5.546809 7.643347 7.198262 5.282617

11 C 7.894260 6.686380 8.822232 8.075708 6.187141

12 C 9.282294 8.022684 10.156536 9.546295 7.571838

13 C 10.422070 9.207699 11.364085 10.540195 8.609277

14 H 2.102521 1.088466 2.577137 3.226323 2.162578

15 H 1.884674 3.205053 2.283175 0.971373 3.701245

16 H 3.470679 2.143323 4.496210 3.812875 1.089311

17 H 2.817679 2.158923 3.836824 2.871202 1.093677

18 H 2.859283 2.171000 4.064691 2.594184 1.089315

19 H 7.067346 5.881953 7.773953 7.551185 5.879319

20 H 6.966450 5.583134 7.771033 7.465716 5.275453

21 H 7.861226 6.632494 8.875611 7.939270 5.897515

22 H 7.935232 6.871696 8.865271 7.999866 6.424471

23 H 9.500872 8.288179 10.287069 9.840795 8.026477

24 H 9.433216 8.082745 10.286577 9.792090 7.609360

25 H 11.385010 10.142794 12.292782 11.558787 9.588661

26 H 10.467155 9.231379 11.472449 10.515505 8.468520

27 H 10.467086 9.356770 11.416640 10.489123 8.783500

6 7 8 9 10

6 S 0.000000

7 C 1.756228 0.000000

8 S 2.944090 1.794448 0.000000

9 S 3.052130 1.719716 3.100976 0.000000

10 C 4.393372 2.851474 1.833941 3.385070 0.000000

11 C 5.623809 4.214712 2.754097 4.831316 1.524284

12 C 6.902148 5.385303 4.159634 5.676564 2.535948

13 C 8.156313 6.716831 5.292772 7.106167 3.899725

14 H 2.432393 3.102965 4.515647 3.285728 5.845888

15 H 4.189460 5.681496 6.285920 6.749002 8.077050

16 H 3.027619 2.702049 3.196248 3.142913 4.552001

17 H 3.823386 4.179016 4.728041 4.655426 6.252381

18 H 3.022483 3.412489 3.472843 4.484582 5.200015

19 H 4.452362 3.045470 2.406036 3.563404 1.092043

20 H 4.663806 2.943386 2.409656 2.900408 1.089213

21 H 5.857274 4.464189 2.925987 5.041408 2.156019

22 H 5.680500 4.525508 2.907728 5.449367 2.158029

23 H 6.966818 5.517284 4.455953 5.817483 2.767871

24 H 7.100230 5.451290 4.464115 5.410714 2.750244

25 H 9.046381 7.558341 6.243310 7.805532 4.709200

26 H 8.383707 6.929142 5.454126 7.279324 4.235070

27 H 8.220613 6.941039 5.390707 7.566201 4.215289

11 12 13 14 15

11 C 0.000000

12 C 1.531093 0.000000

13 C 2.543032 1.527056 0.000000

14 H 7.104402 8.329147 9.597361 0.000000

15 H 8.953124 10.426805 11.412404 3.938470 0.000000

16 H 5.475692 6.777633 7.846329 2.455975 4.770295

17 H 7.100743 8.462598 9.450416 2.538475 3.720760

18 H 5.908723 7.377341 8.291614 3.073772 3.543414

19 H 2.173875 2.795828 4.225709 6.136596 8.372739

20 H 2.170412 2.809737 4.219457 5.702160 8.378459

21 H 1.096121 2.159011 2.758172 7.076852 8.846196

22 H 1.095677 2.154629 2.775011 7.420437 8.821174

23 H 2.154716 1.095779 2.157639 8.569541 10.683247

24 H 2.160031 1.095983 2.157346 8.260464 10.704581

25 H 3.496841 2.179577 1.093412 10.473633 12.433061

26 H 2.836577 2.176486 1.094596 9.629242 11.410379

27 H 2.783066 2.178559 1.094376 9.850038 11.317242

16 17 18 19 20

16 H 0.000000

17 H 1.766836 0.000000

18 H 1.768741 1.771096 0.000000

19 H 5.233710 6.901078 5.828176 0.000000

20 H 4.392728 6.155162 5.386482 1.765871 0.000000

21 H 5.151176 6.707886 5.583228 3.073010 2.508169

22 H 5.867714 7.378571 5.987822 2.525682 3.070479

23 H 7.280197 8.980622 7.854837 2.579926 3.150237

24 H 6.711950 8.437564 7.554754 3.093389 2.577861

25 H 8.787987 10.429037 9.320387 4.895981 4.920104

26 H 7.679887 9.221120 8.138885 4.792335 4.428363

27 H 8.126449 9.658244 8.346430 4.459954 4.768348

21 22 23 24 25

21 H 0.000000

22 H 1.756107 0.000000

23 H 3.059633 2.490838 0.000000

24 H 2.522183 3.060185 1.754610 0.000000

25 H 3.780664 3.761952 2.482047 2.522494 0.000000

26 H 2.607538 3.185569 3.074151 2.500157 1.765624

27 H 3.068339 2.566436 2.546530 3.076541 1.766044

26 27

26 H 0.000000

27 H 1.764065 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.11D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.085263 -0.496124 -0.046682

2 6 0 -2.814408 0.079331 0.494036

3 8 0 -4.958058 0.141301 -0.594006

4 8 0 -4.186979 -1.829318 0.141104

5 6 0 -2.158046 -0.706490 1.614452

6 16 0 -1.650973 0.239296 -1.016995

7 6 0 -0.136299 0.770910 -0.304614

8 16 0 1.060582 -0.561674 -0.196274

9 16 0 0.036160 2.281357 0.499272

10 6 0 2.676279 0.303631 -0.260381

11 6 0 3.806528 -0.692826 -0.030050

12 6 0 5.185191 -0.030968 -0.104059

13 6 0 6.321781 -1.016107 0.159692

14 1 0 -3.016514 1.103945 0.800756

15 1 0 -5.030360 -2.114280 -0.247576

16 1 0 -1.269654 -0.177606 1.957441

17 1 0 -2.841420 -0.807119 2.462392

18 1 0 -1.863812 -1.703425 1.288638

19 1 0 2.762590 0.782575 -1.237990

20 1 0 2.677671 1.083532 0.499972

21 1 0 3.683478 -1.169799 0.949152

22 1 0 3.753154 -1.494219 -0.775321

23 1 0 5.313040 0.421387 -1.093887

24 1 0 5.236014 0.790438 0.619742

25 1 0 7.299316 -0.540631 0.041802

26 1 0 6.269264 -1.416999 1.176878

27 1 0 6.280642 -1.865463 -0.529192

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2882325 0.1951158 0.1820856

Leave Link 202 at Sat Aug 17 17:38:11 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1103.7680915150 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0551216574 Hartrees.

Nuclear repulsion after empirical dispersion term = 1103.7129698576 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2319

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.15D-08

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 89

GePol: Fraction of low-weight points (<1% of avg) = 3.84%

GePol: Cavity surface area = 307.514 Ang\*\*2

GePol: Cavity volume = 319.914 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0055501614 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1103.7074196962 Hartrees.

Leave Link 301 at Sat Aug 17 17:38:11 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.86D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:38:11 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:38:11 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999695 -0.024473 -0.003406 -0.000518 Ang= -2.83 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.63055750688

Leave Link 401 at Sat Aug 17 17:38:12 2019, MaxMem= 1342177280 cpu: 7.5

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16133283.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.77D-15 for 2317.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.49D-15 for 2286 1053.

Iteration 1 A^-1\*A deviation from unit magnitude is 4.66D-15 for 2308.

Iteration 1 A^-1\*A deviation from orthogonality is 1.07D-12 for 1016 1009.

E= -1658.61048214065

DIIS: error= 1.12D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.61048214065 IErMin= 1 ErrMin= 1.12D-02

ErrMax= 1.12D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.37D-01 BMatP= 1.37D-01

IDIUse=3 WtCom= 8.88D-01 WtEn= 1.12D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Recover alternate guess density for next cycle.

RMSDP=2.35D-03 MaxDP=8.00D-02 OVMax= 0.00D+00

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.35D-03 CP: 9.97D-01

E= -1658.22115645537 Delta-E= 0.389325685278 Rises=F Damp=F

Switch densities from cycles 1 and 2 for lowest energy.

DIIS: error= 3.32D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 1 EnMin= -1658.61048214065 IErMin= 1 ErrMin= 1.12D-02

ErrMax= 3.32D-02 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.19D+00 BMatP= 1.37D-01

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.944D+00 0.557D-01

Coeff: 0.944D+00 0.557D-01

Gap= 0.115 Goal= None Shift= 0.000

Gap= 0.136 Goal= None Shift= 0.000

RMSDP=1.38D-02 MaxDP=5.41D-01 DE= 3.89D-01 OVMax= 1.68D-01

Cycle 3 Pass 1 IDiag 1:

RMSU= 8.97D-04 CP: 9.97D-01 1.49D-01

E= -1658.67265130139 Delta-E= -0.451494846023 Rises=F Damp=F

DIIS: error= 2.72D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67265130139 IErMin= 3 ErrMin= 2.72D-03

ErrMax= 2.72D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.64D-02 BMatP= 1.37D-01

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.319D-01 0.711D-01 0.961D+00

Coeff: -0.319D-01 0.711D-01 0.961D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.45D-04 MaxDP=1.06D-02 DE=-4.51D-01 OVMax= 1.62D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.88D-04 CP: 9.97D-01 2.13D-01 9.51D-01

E= -1658.67538005364 Delta-E= -0.002728752246 Rises=F Damp=F

DIIS: error= 2.29D-03 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67538005364 IErMin= 4 ErrMin= 2.29D-03

ErrMax= 2.29D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 5.27D-03 BMatP= 1.64D-02

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.316D-01 0.275D-01 0.504D+00 0.500D+00

Coeff: -0.316D-01 0.275D-01 0.504D+00 0.500D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=1.28D-04 MaxDP=5.88D-03 DE=-2.73D-03 OVMax= 1.13D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 8.53D-05 CP: 9.97D-01 2.14D-01 9.92D-01 5.34D-01

E= -1658.67624347370 Delta-E= -0.000863420060 Rises=F Damp=F

DIIS: error= 9.32D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67624347370 IErMin= 5 ErrMin= 9.32D-04

ErrMax= 9.32D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.01D-03 BMatP= 5.27D-03

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.122D-01 0.438D-02 0.157D+00 0.327D+00 0.523D+00

Coeff: -0.122D-01 0.438D-02 0.157D+00 0.327D+00 0.523D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=5.28D-05 MaxDP=2.10D-03 DE=-8.63D-04 OVMax= 5.00D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.00D-05 CP: 9.97D-01 2.13D-01 1.00D+00 6.43D-01 5.63D-01

E= -1658.67646502729 Delta-E= -0.000221553595 Rises=F Damp=F

DIIS: error= 2.14D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67646502729 IErMin= 6 ErrMin= 2.14D-04

ErrMax= 2.14D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.90D-05 BMatP= 1.01D-03

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.423D-02 0.535D-03 0.479D-01 0.133D+00 0.261D+00 0.561D+00

Coeff: -0.423D-02 0.535D-03 0.479D-01 0.133D+00 0.261D+00 0.561D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=1.04D-05 MaxDP=4.10D-04 DE=-2.22D-04 OVMax= 8.68D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 7.61D-06 CP: 9.97D-01 2.12D-01 1.00D+00 6.58D-01 6.23D-01

CP: 9.06D-01

E= -1658.67647292571 Delta-E= -0.000007898415 Rises=F Damp=F

DIIS: error= 7.78D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67647292571 IErMin= 7 ErrMin= 7.78D-05

ErrMax= 7.78D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 5.82D-06 BMatP= 3.90D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.316D-03-0.504D-03-0.117D-02 0.194D-01 0.574D-01 0.294D+00

Coeff-Com: 0.631D+00

Coeff: -0.316D-03-0.504D-03-0.117D-02 0.194D-01 0.574D-01 0.294D+00

Coeff: 0.631D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=4.93D-06 MaxDP=1.77D-04 DE=-7.90D-06 OVMax= 6.41D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 3.66D-06 CP: 9.97D-01 2.12D-01 1.00D+00 6.70D-01 6.45D-01

CP: 9.57D-01 9.24D-01

E= -1658.67647432204 Delta-E= -0.000001396333 Rises=F Damp=F

DIIS: error= 2.20D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67647432204 IErMin= 8 ErrMin= 2.20D-05

ErrMax= 2.20D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 6.41D-07 BMatP= 5.82D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.389D-03-0.290D-03-0.664D-02-0.728D-02-0.600D-02 0.580D-01

Coeff-Com: 0.270D+00 0.692D+00

Coeff: 0.389D-03-0.290D-03-0.664D-02-0.728D-02-0.600D-02 0.580D-01

Coeff: 0.270D+00 0.692D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=2.82D-06 MaxDP=1.04D-04 DE=-1.40D-06 OVMax= 3.90D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.62D-06 CP: 9.97D-01 2.12D-01 1.00D+00 6.75D-01 6.44D-01

CP: 1.02D+00 1.06D+00 1.08D+00

E= -1658.67647454510 Delta-E= -0.000000223054 Rises=F Damp=F

DIIS: error= 1.16D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67647454510 IErMin= 9 ErrMin= 1.16D-05

ErrMax= 1.16D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.67D-07 BMatP= 6.41D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.270D-03-0.235D-04-0.320D-02-0.804D-02-0.152D-01-0.311D-01

Coeff-Com: 0.230D-02 0.343D+00 0.712D+00

Coeff: 0.270D-03-0.235D-04-0.320D-02-0.804D-02-0.152D-01-0.311D-01

Coeff: 0.230D-02 0.343D+00 0.712D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=1.37D-06 MaxDP=5.70D-05 DE=-2.23D-07 OVMax= 2.19D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 7.17D-07 CP: 9.97D-01 2.12D-01 1.00D+00 6.75D-01 6.49D-01

CP: 1.04D+00 1.12D+00 1.27D+00 9.24D-01

E= -1658.67647460453 Delta-E= -0.000000059435 Rises=F Damp=F

DIIS: error= 6.84D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67647460453 IErMin=10 ErrMin= 6.84D-06

ErrMax= 6.84D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 6.47D-08 BMatP= 1.67D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.104D-03 0.422D-04-0.820D-03-0.414D-02-0.943D-02-0.326D-01

Coeff-Com: -0.521D-01 0.846D-01 0.463D+00 0.551D+00

Coeff: 0.104D-03 0.422D-04-0.820D-03-0.414D-02-0.943D-02-0.326D-01

Coeff: -0.521D-01 0.846D-01 0.463D+00 0.551D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=7.59D-07 MaxDP=3.47D-05 DE=-5.94D-08 OVMax= 9.99D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 3.06D-07 CP: 9.97D-01 2.12D-01 1.00D+00 6.77D-01 6.48D-01

CP: 1.05D+00 1.15D+00 1.36D+00 1.13D+00 7.26D-01

E= -1658.67647462230 Delta-E= -0.000000017773 Rises=F Damp=F

DIIS: error= 1.96D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67647462230 IErMin=11 ErrMin= 1.96D-06

ErrMax= 1.96D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 7.09D-09 BMatP= 6.47D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.103D-04 0.204D-04 0.124D-03-0.719D-03-0.211D-02-0.103D-01

Coeff-Com: -0.266D-01-0.217D-01 0.111D+00 0.290D+00 0.661D+00

Coeff: 0.103D-04 0.204D-04 0.124D-03-0.719D-03-0.211D-02-0.103D-01

Coeff: -0.266D-01-0.217D-01 0.111D+00 0.290D+00 0.661D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=2.34D-07 MaxDP=1.23D-05 DE=-1.78D-08 OVMax= 3.64D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.22D-07 CP: 9.97D-01 2.12D-01 1.00D+00 6.77D-01 6.49D-01

CP: 1.05D+00 1.16D+00 1.38D+00 1.17D+00 8.78D-01

CP: 8.29D-01

E= -1658.67647462472 Delta-E= -0.000000002415 Rises=F Damp=F

DIIS: error= 9.16D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.67647462472 IErMin=12 ErrMin= 9.16D-07

ErrMax= 9.16D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.04D-09 BMatP= 7.09D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.135D-04 0.144D-05 0.210D-03 0.421D-03 0.701D-03 0.119D-02

Coeff-Com: -0.262D-02-0.234D-01-0.340D-01 0.207D-01 0.313D+00 0.724D+00

Coeff: -0.135D-04 0.144D-05 0.210D-03 0.421D-03 0.701D-03 0.119D-02

Coeff: -0.262D-02-0.234D-01-0.340D-01 0.207D-01 0.313D+00 0.724D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=1.05D-07 MaxDP=4.50D-06 DE=-2.41D-09 OVMax= 9.49D-06

Cycle 13 Pass 1 IDiag 1:

RMSU= 5.21D-08 CP: 9.97D-01 2.12D-01 1.00D+00 6.77D-01 6.48D-01

CP: 1.05D+00 1.16D+00 1.39D+00 1.20D+00 9.02D-01

CP: 9.99D-01 9.60D-01

E= -1658.67647462509 Delta-E= -0.000000000372 Rises=F Damp=F

DIIS: error= 2.64D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1658.67647462509 IErMin=13 ErrMin= 2.64D-07

ErrMax= 2.64D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.01D-10 BMatP= 1.04D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.683D-05-0.189D-05 0.634D-04 0.270D-03 0.557D-03 0.195D-02

Coeff-Com: 0.296D-02-0.528D-02-0.292D-01-0.342D-01 0.365D-01 0.274D+00

Coeff-Com: 0.752D+00

Coeff: -0.683D-05-0.189D-05 0.634D-04 0.270D-03 0.557D-03 0.195D-02

Coeff: 0.296D-02-0.528D-02-0.292D-01-0.342D-01 0.365D-01 0.274D+00

Coeff: 0.752D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=3.87D-08 MaxDP=1.40D-06 DE=-3.72D-10 OVMax= 5.70D-06

Cycle 14 Pass 1 IDiag 1:

RMSU= 2.13D-08 CP: 9.97D-01 2.12D-01 1.00D+00 6.77D-01 6.48D-01

CP: 1.05D+00 1.16D+00 1.39D+00 1.20D+00 9.14D-01

CP: 1.06D+00 1.13D+00 9.28D-01

E= -1658.67647462512 Delta-E= -0.000000000034 Rises=F Damp=F

DIIS: error= 8.43D-08 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1658.67647462512 IErMin=14 ErrMin= 8.43D-08

ErrMax= 8.43D-08 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.93D-11 BMatP= 1.01D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.504D-06-0.968D-06-0.225D-04 0.537D-05 0.441D-04 0.431D-03

Coeff-Com: 0.144D-02 0.264D-02-0.300D-02-0.160D-01-0.470D-01-0.594D-01

Coeff-Com: 0.269D+00 0.852D+00

Coeff: 0.504D-06-0.968D-06-0.225D-04 0.537D-05 0.441D-04 0.431D-03

Coeff: 0.144D-02 0.264D-02-0.300D-02-0.160D-01-0.470D-01-0.594D-01

Coeff: 0.269D+00 0.852D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=1.81D-08 MaxDP=1.01D-06 DE=-3.41D-11 OVMax= 1.48D-06

Cycle 15 Pass 1 IDiag 1:

RMSU= 9.17D-09 CP: 9.97D-01 2.12D-01 1.00D+00 6.77D-01 6.48D-01

CP: 1.05D+00 1.16D+00 1.39D+00 1.21D+00 9.15D-01

CP: 1.08D+00 1.19D+00 1.15D+00 1.01D+00

E= -1658.67647462515 Delta-E= -0.000000000026 Rises=F Damp=F

DIIS: error= 3.50D-08 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1658.67647462515 IErMin=15 ErrMin= 3.50D-08

ErrMax= 3.50D-08 0.00D+00 EMaxC= 1.00D+00 BMatC= 4.23D-12 BMatP= 1.93D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.136D-05-0.110D-06-0.208D-04-0.412D-04-0.739D-04-0.154D-03

Coeff-Com: 0.404D-04 0.201D-02 0.430D-02-0.675D-03-0.269D-01-0.784D-01

Coeff-Com: 0.324D-02 0.412D+00 0.684D+00

Coeff: 0.136D-05-0.110D-06-0.208D-04-0.412D-04-0.739D-04-0.154D-03

Coeff: 0.404D-04 0.201D-02 0.430D-02-0.675D-03-0.269D-01-0.784D-01

Coeff: 0.324D-02 0.412D+00 0.684D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=7.02D-09 MaxDP=3.70D-07 DE=-2.64D-11 OVMax= 9.52D-07

Error on total polarization charges = 0.04149

SCF Done: E(UB3LYP) = -1658.67647463 A.U. after 15 cycles

NFock= 15 Conv=0.70D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655264368170D+03 PE=-6.150194377745D+03 EE= 1.732546115253D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.48

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:38:43 2019, MaxMem= 1342177280 cpu: 360.8

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 333

Leave Link 701 at Sat Aug 17 17:38:44 2019, MaxMem= 1342177280 cpu: 10.3

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:38:44 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:38:47 2019, MaxMem= 1342177280 cpu: 36.4

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.49114032D+00-3.04603711D+00 5.49786030D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.003860919 -0.000000315 0.004124545

2 6 0.003641128 -0.000092686 0.000116546

3 8 0.000754651 0.000708852 -0.002236377

4 8 0.001214444 -0.001026912 -0.001296536

5 6 -0.000463336 0.000552741 -0.000903898

6 16 -0.000209270 0.000618422 0.000089151

7 6 -0.000798918 -0.001288459 -0.000604473

8 16 -0.000841139 -0.000488604 0.001105444

9 16 0.000303719 0.000856825 0.000164832

10 6 -0.000018783 -0.000196245 -0.000626817

11 6 0.000549794 0.000198000 0.000057703

12 6 -0.000200489 -0.000261366 -0.000787396

13 6 -0.000176242 -0.000184628 0.000748998

14 1 -0.000792277 0.000266936 -0.000149010

15 1 -0.000374416 0.000020543 -0.000427440

16 1 0.000771242 0.000039786 0.000177587

17 1 -0.000299878 0.000011399 0.000415183

18 1 -0.000008153 -0.000677600 0.000080016

19 1 0.000694483 0.000530637 -0.000319270

20 1 -0.000459375 0.000046170 0.000855650

21 1 -0.000248082 0.000189033 0.000154711

22 1 0.000218342 -0.000422734 -0.000245348

23 1 0.000150619 0.000323550 -0.000267916

24 1 -0.000178045 0.000236545 0.000056297

25 1 0.000459524 0.000111741 0.000110638

26 1 -0.000003514 -0.000166322 0.000199294

27 1 0.000174890 0.000094692 -0.000592113

-------------------------------------------------------------------

Cartesian Forces: Max 0.004124545 RMS 0.000934083

Leave Link 716 at Sat Aug 17 17:38:47 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.001982984 RMS 0.000590280

Search for a local minimum.

Step number 20 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .59028D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 17 18 19 20

DE= 4.99D-04 DEPred=-1.55D-04 R=-3.23D+00

Trust test=-3.23D+00 RLast= 5.98D-01 DXMaxT set to 7.07D-02

ITU= -1 1 -1 1 1 -1 1 -1 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Eigenvalues --- 0.00000 0.00177 0.00297 0.00374 0.00402

Eigenvalues --- 0.00486 0.00921 0.01175 0.02011 0.02379

Eigenvalues --- 0.02905 0.03553 0.03701 0.04221 0.04802

Eigenvalues --- 0.04842 0.04875 0.05181 0.05470 0.05496

Eigenvalues --- 0.05546 0.05660 0.05777 0.05891 0.08281

Eigenvalues --- 0.08318 0.08556 0.11307 0.12113 0.12248

Eigenvalues --- 0.14481 0.15736 0.15778 0.16004 0.16050

Eigenvalues --- 0.16068 0.16348 0.16523 0.17713 0.18995

Eigenvalues --- 0.21361 0.21888 0.22115 0.22881 0.23674

Eigenvalues --- 0.24477 0.24772 0.25620 0.25857 0.26453

Eigenvalues --- 0.28319 0.28864 0.29222 0.29497 0.29771

Eigenvalues --- 0.30389 0.31624 0.32826 0.33820 0.33878

Eigenvalues --- 0.33887 0.33951 0.33982 0.34031 0.34041

Eigenvalues --- 0.34135 0.34360 0.34436 0.34564 0.34654

Eigenvalues --- 0.34862 0.40360 0.52521 0.58436 1.10364

Eigenvalue 1 is 3.61D-07 Eigenvector:

D1 D4 D2 D3 D5

1 0.38082 0.36345 0.36339 0.35631 0.34601

D6 D24 D23 D22 D43

1 0.33894 0.17447 0.12430 -0.10270 -0.10119

En-DIIS/RFO-DIIS IScMMF= 0 using points: 20 19 18 17 16

RFO step: Lambda=-1.30114863D-04.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=T DC= 2.99D-05 SmlDif= 1.00D-05

RMS Error= 0.2286545401D-02 NUsed= 5 EDIIS=T

EnCoef did 100 forward-backward iterations

DidBck=T Rises=T En-DIIS coefs: 0.09070 0.62172 0.27233 0.00000 0.01525

Iteration 1 RMS(Cart)= 0.14303915 RMS(Int)= 0.00625230

Iteration 2 RMS(Cart)= 0.01405072 RMS(Int)= 0.00005364

Iteration 3 RMS(Cart)= 0.00011482 RMS(Int)= 0.00003473

Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00003473

ITry= 1 IFail=0 DXMaxC= 4.61D-01 DCOld= 1.00D+10 DXMaxT= 7.07D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.82740 0.00194 0.00853 -0.00393 0.00460 2.83199

R2 2.28933 0.00072 -0.00207 0.00888 0.00681 2.29614

R3 2.55149 0.00091 0.00142 0.00083 0.00225 2.55375

R4 2.86819 -0.00010 -0.00183 0.00178 -0.00005 2.86814

R5 3.61643 -0.00034 -0.01617 0.01335 -0.00282 3.61361

R6 2.05690 0.00033 0.00054 0.00277 0.00331 2.06021

R7 1.83563 0.00050 0.00074 0.00223 0.00296 1.83859

R8 2.05850 0.00072 0.00196 0.00130 0.00326 2.06176

R9 2.06675 0.00050 0.00135 0.00060 0.00195 2.06870

R10 2.05851 0.00055 0.00131 0.00115 0.00246 2.06097

R11 3.31879 -0.00048 0.00128 -0.00467 -0.00339 3.31540

R12 3.39102 0.00009 -0.00603 0.00294 -0.00309 3.38793

R13 3.24979 0.00082 0.00372 -0.00049 0.00323 3.25302

R14 3.46565 0.00104 0.00851 -0.00016 0.00835 3.47400

R15 2.88048 0.00045 0.00007 0.00131 0.00138 2.88186

R16 2.06366 0.00061 -0.00043 0.00211 0.00168 2.06534

R17 2.05831 0.00069 0.00133 0.00168 0.00300 2.06132

R18 2.89335 0.00025 0.00077 0.00133 0.00210 2.89544

R19 2.07137 0.00005 0.00075 0.00083 0.00157 2.07294

R20 2.07053 0.00045 0.00007 0.00147 0.00154 2.07208

R21 2.88572 0.00048 -0.00026 0.00148 0.00122 2.88694

R22 2.07072 0.00042 0.00091 0.00124 0.00215 2.07288

R23 2.07111 0.00018 0.00039 0.00111 0.00150 2.07260

R24 2.06625 0.00045 0.00104 0.00099 0.00203 2.06828

R25 2.06849 0.00025 0.00043 0.00136 0.00178 2.07027

R26 2.06807 0.00037 0.00061 0.00133 0.00194 2.07001

A1 2.18077 -0.00077 -0.00330 -0.00146 -0.00471 2.17606

A2 1.97523 0.00048 0.00021 0.00605 0.00631 1.98154

A3 2.12715 0.00031 0.00252 -0.00460 -0.00202 2.12514

A4 2.02080 0.00077 0.00316 0.00563 0.00879 2.02959

A5 1.83711 -0.00109 0.00063 -0.00928 -0.00866 1.82846

A6 1.88197 -0.00055 -0.00823 0.00317 -0.00508 1.87689

A7 1.94253 0.00055 0.00116 -0.00005 0.00114 1.94367

A8 1.93869 0.00012 -0.00005 0.00124 0.00120 1.93989

A9 1.83039 0.00007 0.00318 -0.00178 0.00138 1.83178

A10 1.87489 -0.00029 -0.00080 -0.00329 -0.00409 1.87079

A11 1.91107 0.00026 -0.00143 0.00044 -0.00099 1.91008

A12 1.92811 -0.00018 0.00103 -0.00082 0.00022 1.92832

A13 1.94964 0.00036 0.00308 -0.00247 0.00061 1.95025

A14 1.88614 -0.00003 -0.00178 0.00284 0.00106 1.88720

A15 1.89466 -0.00025 -0.00096 -0.00060 -0.00157 1.89310

A16 1.89280 -0.00017 -0.00012 0.00079 0.00067 1.89347

A17 1.80221 0.00067 -0.00775 0.00388 -0.00387 1.79834

A18 1.95514 0.00138 0.01255 0.00124 0.01358 1.96872

A19 2.14358 -0.00039 -0.00164 -0.00058 -0.00243 2.14114

A20 2.16173 -0.00072 -0.00653 0.00460 -0.00214 2.15959

A21 1.80814 -0.00198 -0.01189 -0.00070 -0.01259 1.79555

A22 1.91721 0.00157 0.00922 0.00383 0.01306 1.93027

A23 1.88374 0.00016 -0.00913 0.00545 -0.00369 1.88005

A24 1.89079 -0.00106 0.00439 -0.00592 -0.00152 1.88928

A25 1.94268 -0.00084 -0.00266 -0.00137 -0.00404 1.93865

A26 1.94083 -0.00013 -0.00191 -0.00055 -0.00244 1.93839

A27 1.88683 0.00028 -0.00014 -0.00149 -0.00165 1.88518

A28 1.95820 -0.00050 -0.00470 -0.00236 -0.00706 1.95113

A29 1.91369 -0.00023 0.00408 -0.00174 0.00234 1.91603

A30 1.91690 0.00052 -0.00178 0.00339 0.00160 1.91851

A31 1.90961 0.00033 -0.00326 0.00118 -0.00209 1.90752

A32 1.90409 -0.00003 0.00571 -0.00227 0.00345 1.90754

A33 1.85865 -0.00005 0.00022 0.00201 0.00222 1.86088

A34 1.96382 0.00030 0.00301 0.00092 0.00393 1.96775

A35 1.90411 0.00019 0.00221 -0.00086 0.00134 1.90545

A36 1.91114 -0.00041 -0.00357 -0.00186 -0.00543 1.90571

A37 1.91293 -0.00011 0.00021 0.00049 0.00070 1.91363

A38 1.91232 0.00003 0.00005 -0.00064 -0.00060 1.91172

A39 1.85642 -0.00002 -0.00221 0.00202 -0.00019 1.85623

A40 1.94579 0.00014 -0.00028 -0.00111 -0.00139 1.94440

A41 1.94021 0.00011 0.00178 -0.00172 0.00006 1.94027

A42 1.94334 -0.00022 0.00101 -0.00108 -0.00007 1.94327

A43 1.87796 -0.00011 -0.00136 0.00181 0.00045 1.87841

A44 1.87888 -0.00010 -0.00184 0.00165 -0.00020 1.87869

A45 1.87435 0.00017 0.00052 0.00071 0.00124 1.87558

D1 2.70333 0.00110 -0.01872 0.10568 0.08697 2.79031

D2 -1.42680 0.00147 -0.01470 0.10221 0.08750 -1.33930

D3 0.52003 0.00083 -0.01426 0.09732 0.08309 0.60311

D4 -0.42992 -0.00123 -0.06083 0.10751 0.04667 -0.38325

D5 1.72313 -0.00085 -0.05681 0.10404 0.04720 1.77033

D6 -2.61323 -0.00150 -0.05637 0.09915 0.04279 -2.57044

D7 -3.12977 0.00129 0.02637 0.00107 0.02741 -3.10236

D8 0.01988 -0.00095 -0.01441 0.00282 -0.01156 0.00832

D9 -3.10006 -0.00025 -0.01286 0.00101 -0.01185 -3.11191

D10 -1.02477 -0.00025 -0.01531 0.00428 -0.01103 -1.03580

D11 1.08376 -0.00034 -0.01267 0.00306 -0.00962 1.07414

D12 1.08638 0.00020 -0.01693 0.00928 -0.00766 1.07872

D13 -3.12151 0.00021 -0.01938 0.01254 -0.00684 -3.12835

D14 -1.01298 0.00011 -0.01674 0.01132 -0.00543 -1.01841

D15 -0.94619 -0.00031 -0.02160 0.01074 -0.01085 -0.95704

D16 1.12910 -0.00030 -0.02405 0.01401 -0.01003 1.11907

D17 -3.04555 -0.00039 -0.02141 0.01279 -0.00862 -3.05417

D18 -3.05149 -0.00093 -0.06129 -0.01619 -0.07749 -3.12898

D19 -0.84931 -0.00038 -0.05621 -0.01557 -0.07178 -0.92109

D20 1.24849 0.00010 -0.05370 -0.01519 -0.06889 1.17960

D21 1.80540 0.00026 0.01890 -0.00689 0.01200 1.81740

D22 -1.11644 -0.00095 -0.00388 -0.03252 -0.03638 -1.15282

D23 2.66419 -0.00095 -0.06882 0.01253 -0.05633 2.60785

D24 -0.69985 0.00033 -0.04511 0.03770 -0.00737 -0.70721

D25 3.03801 0.00028 0.19769 -0.00544 0.19223 -3.05295

D26 -1.12419 0.00029 0.19425 -0.00142 0.19284 -0.93135

D27 0.91489 0.00015 0.19151 -0.00339 0.18814 1.10303

D28 3.11906 0.00036 0.05666 -0.01473 0.04193 -3.12219

D29 -1.03847 0.00027 0.05220 -0.01603 0.03618 -1.00230

D30 0.99818 0.00037 0.05381 -0.01263 0.04118 1.03936

D31 1.03376 -0.00033 0.06376 -0.02316 0.04060 1.07436

D32 -3.12378 -0.00041 0.05930 -0.02446 0.03484 -3.08893

D33 -1.08712 -0.00031 0.06090 -0.02106 0.03985 -1.04728

D34 -1.07119 -0.00002 0.06703 -0.01996 0.04706 -1.02413

D35 1.05446 -0.00011 0.06257 -0.02126 0.04131 1.09577

D36 3.09111 -0.00001 0.06417 -0.01786 0.04631 3.13743

D37 3.11700 -0.00037 0.02929 -0.02833 0.00096 3.11796

D38 -1.03929 -0.00017 0.03314 -0.02771 0.00544 -1.03385

D39 0.98590 -0.00032 0.02974 -0.02681 0.00293 0.98884

D40 0.98902 0.00003 0.02952 -0.02538 0.00414 0.99316

D41 3.11592 0.00023 0.03337 -0.02475 0.00862 3.12454

D42 -1.14208 0.00008 0.02997 -0.02385 0.00611 -1.13596

D43 -1.03798 -0.00007 0.02788 -0.02718 0.00070 -1.03728

D44 1.08892 0.00013 0.03173 -0.02655 0.00518 1.09410

D45 3.11410 -0.00002 0.02833 -0.02565 0.00268 3.11678

D46 3.07999 0.00029 0.05294 -0.01436 0.03857 3.11856

D47 -1.10783 0.00032 0.05224 -0.01399 0.03825 -1.06958

D48 0.98132 0.00047 0.05478 -0.01496 0.03981 1.02113

D49 0.95810 -0.00008 0.04793 -0.01423 0.03370 0.99180

D50 3.05347 -0.00005 0.04723 -0.01385 0.03338 3.08685

D51 -1.14057 0.00010 0.04977 -0.01483 0.03494 -1.10563

D52 -1.07276 -0.00001 0.05044 -0.01658 0.03387 -1.03889

D53 1.02260 0.00002 0.04974 -0.01620 0.03355 1.05615

D54 3.11175 0.00017 0.05229 -0.01718 0.03511 -3.13633

Item Value Threshold Converged?

Maximum Force 0.001983 0.000450 NO

RMS Force 0.000590 0.000300 NO

Maximum Displacement 0.461247 0.001800 NO

RMS Displacement 0.141219 0.001200 NO

Predicted change in Energy=-3.181162D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:38:47 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.107633 -0.403457 -0.174491

2 6 0 -2.835428 0.052409 0.473246

3 8 0 -4.862591 0.316256 -0.797741

4 8 0 -4.337577 -1.728217 -0.038940

5 6 0 -2.284541 -0.837308 1.572563

6 16 0 -1.591336 0.230250 -0.968031

7 6 0 -0.120463 0.742264 -0.160309

8 16 0 1.085399 -0.576048 -0.011516

9 16 0 0.022979 2.263134 0.633214

10 6 0 2.686657 0.325460 -0.064680

11 6 0 3.854389 -0.655335 -0.075531

12 6 0 5.204850 0.068284 -0.092132

13 6 0 6.390982 -0.894248 -0.069933

14 1 0 -2.995980 1.068847 0.833313

15 1 0 -5.159590 -1.928013 -0.519558

16 1 0 -1.379546 -0.387890 1.984100

17 1 0 -3.012876 -0.940012 2.383344

18 1 0 -2.037846 -1.832618 1.201151

19 1 0 2.688101 0.948230 -0.962820

20 1 0 2.736459 0.984675 0.802962

21 1 0 3.801982 -1.304701 0.807011

22 1 0 3.783732 -1.310709 -0.951770

23 1 0 5.262201 0.703626 -0.984478

24 1 0 5.263319 0.742285 0.771128

25 1 0 7.343144 -0.355726 -0.105762

26 1 0 6.388756 -1.503924 0.840284

27 1 0 6.364617 -1.579152 -0.924402

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.498626 0.000000

3 O 1.215067 2.407159 0.000000

4 O 1.351384 2.385249 2.243054 0.000000

5 C 2.562048 1.517752 3.687193 2.757828 0.000000

6 S 2.713493 1.912242 3.276814 3.498663 2.841624

7 C 4.148543 2.871990 4.803706 4.888974 3.190788

8 S 5.198455 4.000355 6.065719 5.544088 3.732835

9 S 4.982475 3.617097 5.450392 5.949549 3.977407

10 C 6.834161 5.554939 7.584762 7.318341 5.361474

11 C 7.966620 6.749497 8.800643 8.262005 6.358914

12 C 9.324788 8.060147 10.095185 9.710209 7.725431

13 C 10.510601 9.290740 11.341867 10.760969 8.829821

14 H 2.102171 1.090217 2.590554 3.222465 2.164732

15 H 1.884133 3.210834 2.280863 0.972942 3.719208

16 H 3.478825 2.143861 4.512878 3.826110 1.091035

17 H 2.833532 2.159829 3.888310 2.871160 1.094708

18 H 2.866864 2.172397 4.073379 2.614859 1.090617

19 H 6.973559 5.777037 7.578892 7.574766 5.860331

20 H 7.051519 5.658954 7.794524 7.623029 5.396513

21 H 8.021072 6.782946 8.959775 8.194353 6.152259

22 H 7.981286 6.906666 8.799412 8.183107 6.589408

23 H 9.469715 8.253523 10.133921 9.948047 8.115802

24 H 9.487975 8.133534 10.255580 9.946698 7.752909

25 H 11.451083 10.203193 12.243789 11.761269 9.784733

26 H 10.602594 9.361756 11.514730 10.764645 8.729645

27 H 10.564689 9.447552 11.386783 10.739796 9.032890

6 7 8 9 10

6 S 0.000000

7 C 1.754435 0.000000

8 S 2.954648 1.792815 0.000000

9 S 3.050019 1.721424 3.099252 0.000000

10 C 4.373366 2.839506 1.838361 3.367019 0.000000

11 C 5.588984 4.214251 2.770865 4.868211 1.525016

12 C 6.854311 5.368226 4.170316 5.674088 2.531440

13 C 8.111010 6.714555 5.315438 7.142474 3.899966

14 H 2.433332 3.059827 4.480744 3.252764 5.800981

15 H 4.194242 5.714214 6.409820 6.764142 8.176102

16 H 3.023579 2.731488 3.177080 3.289361 4.608728

17 H 3.823873 4.203127 4.760639 4.747580 6.330791

18 H 3.026573 3.487112 3.578294 4.620036 5.346079

19 H 4.339251 2.928220 2.407707 3.373302 1.092932

20 H 4.736600 3.024674 2.413551 3.004370 1.090802

21 H 5.881728 4.528945 2.929291 5.200049 2.158985

22 H 5.591617 4.481500 2.950391 5.424738 2.160451

23 H 6.869885 5.445532 4.475477 5.700740 2.760881

24 H 7.090356 5.463761 4.450343 5.458311 2.740713

25 H 8.995099 7.544135 6.262331 7.809566 4.706227

26 H 8.364164 6.958195 5.450882 7.399778 4.227427

27 H 8.159230 6.930301 5.450663 7.576655 4.230137

11 12 13 14 15

11 C 0.000000

12 C 1.532202 0.000000

13 C 2.547825 1.527701 0.000000

14 H 7.122244 8.313313 9.632479 0.000000

15 H 9.114202 10.563593 11.605453 3.936069 0.000000

16 H 5.630957 6.919039 8.053357 2.461555 4.788425

17 H 7.299756 8.641508 9.718704 2.537400 3.743176

18 H 6.142829 7.598859 8.575625 3.077633 3.565841

19 H 2.172309 2.804715 4.231229 5.962333 8.369916

20 H 2.170519 2.780993 4.200933 5.733137 8.519413

21 H 1.096952 2.159070 2.764132 7.200466 9.080642

22 H 1.096495 2.158744 2.783671 7.403600 8.975014

23 H 2.157520 1.096919 2.159570 8.463764 10.758968

24 H 2.157604 1.096774 2.158066 8.265986 10.836669

25 H 3.501726 2.179970 1.094487 10.478967 12.608000

26 H 2.825215 2.177813 1.095539 9.731006 11.635863

27 H 2.806290 2.179858 1.095402 9.885456 11.536591

16 17 18 19 20

16 H 0.000000

17 H 1.769746 0.000000

18 H 1.770200 1.773417 0.000000

19 H 5.197625 6.874838 5.894952 0.000000

20 H 4.496723 6.265531 5.557849 1.766819 0.000000

21 H 5.392060 7.004292 5.876873 3.073879 2.525193

22 H 6.010854 7.579860 6.228823 2.510644 3.073215

23 H 7.356403 9.084089 8.031201 2.585786 3.106977

24 H 6.846623 8.597951 7.753842 3.111388 2.538659

25 H 8.969608 10.666967 9.586042 4.909610 4.883032

26 H 7.930975 9.544093 8.440728 4.791565 4.419706

27 H 8.357664 9.964289 8.670848 4.461604 4.766606

21 22 23 24 25

21 H 0.000000

22 H 1.758886 0.000000

23 H 3.061871 2.498897 0.000000

24 H 2.515342 3.061427 1.756032 0.000000

25 H 3.778033 3.781155 2.494933 2.510027 0.000000

26 H 2.594648 3.167797 3.077688 2.513334 1.767545

27 H 3.104869 2.594952 2.535746 3.078433 1.767614

26 27

26 H 0.000000

27 H 1.766453 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 6.46D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.113951 -0.422878 -0.126982

2 6 0 -2.836054 0.078374 0.474357

3 8 0 -4.869690 0.247188 -0.802451

4 8 0 -4.348461 -1.731172 0.117170

5 6 0 -2.282225 -0.721493 1.639285

6 16 0 -1.599888 0.132781 -0.983588

7 6 0 -0.122144 0.702102 -0.228481

8 16 0 1.079219 -0.605200 0.020264

9 16 0 0.032219 2.281796 0.437882

10 6 0 2.683781 0.281725 -0.115064

11 6 0 3.847432 -0.701990 -0.052671

12 6 0 5.200699 0.011749 -0.135677

13 6 0 6.383021 -0.951161 -0.041933

14 1 0 -2.990318 1.121444 0.751450

15 1 0 -5.174137 -1.965658 -0.340970

16 1 0 -1.372967 -0.244209 2.007803

17 1 0 -3.006111 -0.754622 2.459820

18 1 0 -2.041801 -1.744818 1.348682

19 1 0 2.682386 0.829386 -1.060879

20 1 0 2.741447 1.009079 0.695787

21 1 0 3.797663 -1.277196 0.880048

22 1 0 3.768876 -1.426119 -0.872285

23 1 0 5.255296 0.572157 -1.077055

24 1 0 5.267066 0.753443 0.669555

25 1 0 7.337132 -0.421661 -0.126805

26 1 0 6.383759 -1.484786 0.914858

27 1 0 6.348766 -1.703154 -0.837697

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3207528 0.1924116 0.1802285

Leave Link 202 at Sat Aug 17 17:38:47 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1101.4426326397 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0549185029 Hartrees.

Nuclear repulsion after empirical dispersion term = 1101.3877141368 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2310

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.31D-11

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 86

GePol: Fraction of low-weight points (<1% of avg) = 3.72%

GePol: Cavity surface area = 309.636 Ang\*\*2

GePol: Cavity volume = 320.624 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057855121 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1101.3819286247 Hartrees.

Leave Link 301 at Sat Aug 17 17:38:47 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 294 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:38:47 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:38:47 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999993 0.002385 0.002223 0.001762 Ang= 0.42 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7553 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.62961187584

Leave Link 401 at Sat Aug 17 17:38:48 2019, MaxMem= 1342177280 cpu: 7.5

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16008300.

Iteration 1 A\*A^-1 deviation from unit magnitude is 4.66D-15 for 2302.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.52D-15 for 945 32.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.33D-15 for 191.

Iteration 1 A^-1\*A deviation from orthogonality is 2.78D-12 for 596 587.

E= -1658.63035496639

DIIS: error= 8.43D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.63035496639 IErMin= 1 ErrMin= 8.43D-03

ErrMax= 8.43D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.04D-01 BMatP= 1.04D-01

IDIUse=3 WtCom= 9.16D-01 WtEn= 8.43D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.429 Goal= None Shift= 0.000

Gap= 0.484 Goal= None Shift= 0.000

GapD= 0.429 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=7.26D-04 MaxDP=1.72D-02 OVMax= 4.02D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 7.25D-04 CP: 9.98D-01

E= -1658.67630899493 Delta-E= -0.045954028541 Rises=F Damp=F

DIIS: error= 1.00D-03 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67630899493 IErMin= 2 ErrMin= 1.00D-03

ErrMax= 1.00D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.79D-03 BMatP= 1.04D-01

IDIUse=3 WtCom= 9.90D-01 WtEn= 1.00D-02

Coeff-Com: -0.628D-01 0.106D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.622D-01 0.106D+01

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=1.18D-04 MaxDP=3.51D-03 DE=-4.60D-02 OVMax= 6.31D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.11D-04 CP: 9.98D-01 1.06D+00

E= -1658.67672416062 Delta-E= -0.000415165691 Rises=F Damp=F

DIIS: error= 1.04D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67672416062 IErMin= 2 ErrMin= 1.00D-03

ErrMax= 1.04D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.08D-03 BMatP= 1.79D-03

IDIUse=3 WtCom= 9.90D-01 WtEn= 1.04D-02

Coeff-Com: -0.361D-01 0.492D+00 0.544D+00

Coeff-En: 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.357D-01 0.487D+00 0.549D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.81D-05 MaxDP=2.38D-03 DE=-4.15D-04 OVMax= 5.71D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 4.99D-05 CP: 9.98D-01 1.08D+00 6.10D-01

E= -1658.67687107514 Delta-E= -0.000146914518 Rises=F Damp=F

DIIS: error= 8.25D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67687107514 IErMin= 4 ErrMin= 8.25D-04

ErrMax= 8.25D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.16D-04 BMatP= 1.08D-03

IDIUse=3 WtCom= 9.92D-01 WtEn= 8.25D-03

Coeff-Com: -0.128D-01 0.163D+00 0.380D+00 0.470D+00

Coeff-En: 0.000D+00 0.000D+00 0.290D+00 0.710D+00

Coeff: -0.127D-01 0.162D+00 0.379D+00 0.472D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.85D-05 MaxDP=1.00D-03 DE=-1.47D-04 OVMax= 2.74D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.74D-05 CP: 9.98D-01 1.09D+00 7.05D-01 6.07D-01

E= -1658.67695303802 Delta-E= -0.000081962877 Rises=F Damp=F

DIIS: error= 1.40D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67695303802 IErMin= 5 ErrMin= 1.40D-04

ErrMax= 1.40D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.41D-05 BMatP= 4.16D-04

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.40D-03

Coeff-Com: -0.313D-02 0.343D-01 0.141D+00 0.232D+00 0.596D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.312D-02 0.342D-01 0.141D+00 0.232D+00 0.596D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.62D-06 MaxDP=2.12D-04 DE=-8.20D-05 OVMax= 4.85D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 5.09D-06 CP: 9.98D-01 1.09D+00 7.26D-01 6.67D-01 8.89D-01

E= -1658.67695600344 Delta-E= -0.000002965416 Rises=F Damp=F

DIIS: error= 4.64D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67695600344 IErMin= 6 ErrMin= 4.64D-05

ErrMax= 4.64D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.28D-06 BMatP= 1.41D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.813D-03-0.153D-01 0.338D-02 0.360D-01 0.314D+00 0.661D+00

Coeff: 0.813D-03-0.153D-01 0.338D-02 0.360D-01 0.314D+00 0.661D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.28D-06 MaxDP=1.29D-04 DE=-2.97D-06 OVMax= 3.17D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.39D-06 CP: 9.98D-01 1.09D+00 7.37D-01 6.96D-01 9.46D-01

CP: 8.77D-01

E= -1658.67695657861 Delta-E= -0.000000575177 Rises=F Damp=F

DIIS: error= 1.34D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67695657861 IErMin= 7 ErrMin= 1.34D-05

ErrMax= 1.34D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.35D-07 BMatP= 2.28D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.667D-03-0.103D-01-0.118D-01-0.556D-02 0.833D-01 0.300D+00

Coeff-Com: 0.644D+00

Coeff: 0.667D-03-0.103D-01-0.118D-01-0.556D-02 0.833D-01 0.300D+00

Coeff: 0.644D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.44D-06 MaxDP=4.74D-05 DE=-5.75D-07 OVMax= 1.56D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.08D-06 CP: 9.98D-01 1.09D+00 7.40D-01 6.96D-01 9.87D-01

CP: 9.79D-01 1.02D+00

E= -1658.67695663847 Delta-E= -0.000000059856 Rises=F Damp=F

DIIS: error= 7.24D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67695663847 IErMin= 8 ErrMin= 7.24D-06

ErrMax= 7.24D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.56D-08 BMatP= 2.35D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.217D-03-0.258D-02-0.805D-02-0.119D-01-0.225D-01 0.321D-01

Coeff-Com: 0.416D+00 0.597D+00

Coeff: 0.217D-03-0.258D-02-0.805D-02-0.119D-01-0.225D-01 0.321D-01

Coeff: 0.416D+00 0.597D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=8.41D-07 MaxDP=3.14D-05 DE=-5.99D-08 OVMax= 8.83D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 4.11D-07 CP: 9.98D-01 1.09D+00 7.40D-01 7.04D-01 9.97D-01

CP: 1.04D+00 1.21D+00 7.57D-01

E= -1658.67695666680 Delta-E= -0.000000028328 Rises=F Damp=F

DIIS: error= 2.53D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67695666680 IErMin= 9 ErrMin= 2.53D-06

ErrMax= 2.53D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.41D-08 BMatP= 9.56D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.217D-04 0.820D-03-0.217D-02-0.595D-02-0.310D-01-0.457D-01

Coeff-Com: 0.993D-01 0.330D+00 0.655D+00

Coeff: -0.217D-04 0.820D-03-0.217D-02-0.595D-02-0.310D-01-0.457D-01

Coeff: 0.993D-01 0.330D+00 0.655D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.49D-07 MaxDP=1.49D-05 DE=-2.83D-08 OVMax= 4.19D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.54D-07 CP: 9.98D-01 1.09D+00 7.41D-01 7.04D-01 1.00D+00

CP: 1.06D+00 1.28D+00 9.21D-01 8.21D-01

E= -1658.67695667093 Delta-E= -0.000000004138 Rises=F Damp=F

DIIS: error= 1.18D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67695667093 IErMin=10 ErrMin= 1.18D-06

ErrMax= 1.18D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.60D-09 BMatP= 1.41D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.438D-04 0.853D-03 0.342D-04-0.157D-02-0.134D-01-0.301D-01

Coeff-Com: -0.145D-01 0.842D-01 0.372D+00 0.603D+00

Coeff: -0.438D-04 0.853D-03 0.342D-04-0.157D-02-0.134D-01-0.301D-01

Coeff: -0.145D-01 0.842D-01 0.372D+00 0.603D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.30D-07 MaxDP=6.18D-06 DE=-4.14D-09 OVMax= 1.47D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 5.73D-08 CP: 9.98D-01 1.09D+00 7.41D-01 7.05D-01 1.00D+00

CP: 1.07D+00 1.31D+00 9.40D-01 9.42D-01 7.59D-01

E= -1658.67695667163 Delta-E= -0.000000000695 Rises=F Damp=F

DIIS: error= 3.31D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67695667163 IErMin=11 ErrMin= 3.31D-07

ErrMax= 3.31D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.60D-10 BMatP= 2.60D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.154D-04 0.254D-03 0.183D-03-0.155D-03-0.235D-02-0.754D-02

Coeff-Com: -0.159D-01 0.208D-02 0.859D-01 0.249D+00 0.689D+00

Coeff: -0.154D-04 0.254D-03 0.183D-03-0.155D-03-0.235D-02-0.754D-02

Coeff: -0.159D-01 0.208D-02 0.859D-01 0.249D+00 0.689D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.03D-08 MaxDP=1.66D-06 DE=-6.95D-10 OVMax= 3.87D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 2.60D-08 CP: 9.98D-01 1.09D+00 7.41D-01 7.05D-01 1.00D+00

CP: 1.07D+00 1.31D+00 9.53D-01 9.71D-01 8.65D-01

CP: 8.79D-01

E= -1658.67695667166 Delta-E= -0.000000000030 Rises=F Damp=F

DIIS: error= 1.27D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.67695667166 IErMin=12 ErrMin= 1.27D-07

ErrMax= 1.27D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.80D-11 BMatP= 1.60D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.914D-07-0.256D-04 0.868D-04 0.201D-03 0.127D-02 0.175D-02

Coeff-Com: -0.544D-02-0.142D-01-0.236D-01 0.185D-01 0.364D+00 0.658D+00

Coeff: 0.914D-07-0.256D-04 0.868D-04 0.201D-03 0.127D-02 0.175D-02

Coeff: -0.544D-02-0.142D-01-0.236D-01 0.185D-01 0.364D+00 0.658D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.64D-08 MaxDP=7.18D-07 DE=-3.05D-11 OVMax= 1.79D-06

Cycle 13 Pass 1 IDiag 1:

RMSU= 8.47D-09 CP: 9.98D-01 1.09D+00 7.41D-01 7.05D-01 1.00D+00

CP: 1.07D+00 1.32D+00 9.55D-01 9.85D-01 8.93D-01

CP: 1.04D+00 9.20D-01

E= -1658.67695667169 Delta-E= -0.000000000029 Rises=F Damp=F

DIIS: error= 4.27D-08 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1658.67695667169 IErMin=13 ErrMin= 4.27D-08

ErrMax= 4.27D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.97D-12 BMatP= 3.80D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.155D-05-0.333D-04 0.965D-05 0.863D-04 0.636D-03 0.133D-02

Coeff-Com: -0.260D-04-0.450D-02-0.168D-01-0.200D-01 0.359D-01 0.192D+00

Coeff-Com: 0.811D+00

Coeff: 0.155D-05-0.333D-04 0.965D-05 0.863D-04 0.636D-03 0.133D-02

Coeff: -0.260D-04-0.450D-02-0.168D-01-0.200D-01 0.359D-01 0.192D+00

Coeff: 0.811D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.62D-09 MaxDP=2.24D-07 DE=-2.91D-11 OVMax= 6.42D-07

Error on total polarization charges = 0.04167

SCF Done: E(UB3LYP) = -1658.67695667 A.U. after 13 cycles

NFock= 13 Conv=0.56D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655207392484D+03 PE=-6.145505757499D+03 EE= 1.730239479719D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.63

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:39:15 2019, MaxMem= 1342177280 cpu: 314.0

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 336

Leave Link 701 at Sat Aug 17 17:39:16 2019, MaxMem= 1342177280 cpu: 10.2

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:39:16 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:39:19 2019, MaxMem= 1342177280 cpu: 36.1

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.39642474D+00-2.96451189D+00 5.72394241D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.004538552 0.002365457 -0.002624515

2 6 0.000968281 -0.000470949 0.000649656

3 8 0.003103348 -0.002754729 0.002551976

4 8 0.000302041 0.000294376 -0.000376210

5 6 -0.000308969 0.000688643 -0.000849506

6 16 -0.000029099 0.000413243 0.000398297

7 6 -0.000456219 -0.000152892 -0.000209409

8 16 0.000549149 0.000111426 0.000185136

9 16 0.000107981 -0.000242411 0.000108401

10 6 -0.000111579 0.000457771 -0.000025771

11 6 0.000022358 -0.000153056 -0.000035783

12 6 -0.000233907 0.000127249 0.000045690

13 6 -0.000239761 -0.000262444 0.000061111

14 1 0.000072859 -0.000309992 -0.000558489

15 1 0.000619453 0.000183389 0.000388975

16 1 -0.000044259 -0.000279971 0.000152250

17 1 0.000338699 0.000136928 -0.000002063

18 1 -0.000193647 0.000019336 0.000237881

19 1 -0.000043504 -0.000178735 0.000193387

20 1 0.000006866 -0.000363402 -0.000271465

21 1 0.000031768 0.000215779 -0.000197928

22 1 -0.000074677 0.000067347 0.000329561

23 1 -0.000036066 -0.000094063 0.000374232

24 1 0.000160232 -0.000078084 -0.000272562

25 1 -0.000163881 -0.000235683 0.000031642

26 1 0.000119773 0.000137773 -0.000382030

27 1 0.000071311 0.000357692 0.000097536

-------------------------------------------------------------------

Cartesian Forces: Max 0.004538552 RMS 0.000888544

Leave Link 716 at Sat Aug 17 17:39:19 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.004866240 RMS 0.000516722

Search for a local minimum.

Step number 21 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .51672D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 5 8 10 11 12

13 14 15 16 17

18 19 20 21

DE= -4.82D-04 DEPred=-3.18D-04 R= 1.52D+00

TightC=F SS= 1.41D+00 RLast= 4.34D-01 DXNew= 1.1892D-01 1.3022D+00

Trust test= 1.52D+00 RLast= 4.34D-01 DXMaxT set to 1.19D-01

ITU= 1 -1 1 -1 1 1 -1 1 -1 1 1 -1 0 0 -1 0 0 -1 -1 0

ITU= 0

Eigenvalues --- 0.00001 0.00157 0.00173 0.00380 0.00384

Eigenvalues --- 0.00443 0.00779 0.01185 0.01770 0.02273

Eigenvalues --- 0.02408 0.03552 0.03769 0.04204 0.04747

Eigenvalues --- 0.04831 0.04881 0.05125 0.05432 0.05480

Eigenvalues --- 0.05513 0.05672 0.05800 0.05953 0.08214

Eigenvalues --- 0.08363 0.08603 0.11324 0.12073 0.12235

Eigenvalues --- 0.14214 0.14763 0.15814 0.16001 0.16022

Eigenvalues --- 0.16051 0.16077 0.16365 0.17181 0.18457

Eigenvalues --- 0.20167 0.21916 0.22034 0.22571 0.23981

Eigenvalues --- 0.24179 0.24760 0.25581 0.25915 0.27114

Eigenvalues --- 0.28304 0.28775 0.29260 0.29486 0.29830

Eigenvalues --- 0.30640 0.31927 0.32552 0.33653 0.33877

Eigenvalues --- 0.33894 0.33943 0.33965 0.34032 0.34034

Eigenvalues --- 0.34119 0.34274 0.34432 0.34576 0.34667

Eigenvalues --- 0.34705 0.37671 0.52532 0.55325 1.08178

Eigenvalue 1 is 6.82D-06 Eigenvector:

D6 D4 D20 D5 D18

1 0.28444 0.26218 0.25599 0.24101 0.23175

D3 D19 D1 D17 D2

1 0.22240 0.20835 0.20014 -0.18234 0.17897

En-DIIS/RFO-DIIS IScMMF= 0 using points: 21 20 19 18 17

RFO step: Lambda=-5.57469508D-05.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= -2.82D-04 SmlDif= 1.00D-05

RMS Error= 0.2127304573D-02 NUsed= 5 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: -0.11355 0.29423 1.47896 0.11712 -0.77676

Iteration 1 RMS(Cart)= 0.10240774 RMS(Int)= 0.00308345

Iteration 2 RMS(Cart)= 0.00831448 RMS(Int)= 0.00007714

Iteration 3 RMS(Cart)= 0.00003014 RMS(Int)= 0.00007655

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00007655

ITry= 1 IFail=0 DXMaxC= 5.15D-01 DCOld= 1.00D+10 DXMaxT= 1.19D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83199 0.00045 0.00307 0.02226 0.02532 2.85731

R2 2.29614 -0.00487 -0.00707 -0.00558 -0.01264 2.28350

R3 2.55375 -0.00062 -0.00064 0.00920 0.00856 2.56231

R4 2.86814 -0.00077 -0.00114 -0.00412 -0.00526 2.86288

R5 3.61361 -0.00056 -0.01000 0.00732 -0.00268 3.61093

R6 2.06021 -0.00049 -0.00216 0.00095 -0.00121 2.05900

R7 1.83859 -0.00075 -0.00175 0.00075 -0.00100 1.83759

R8 2.06176 -0.00009 -0.00105 0.00018 -0.00087 2.06088

R9 2.06870 -0.00024 -0.00042 0.00216 0.00174 2.07044

R10 2.06097 -0.00015 -0.00096 0.00231 0.00135 2.06232

R11 3.31540 -0.00029 0.00408 -0.00254 0.00155 3.31695

R12 3.38793 0.00000 -0.00221 -0.01145 -0.01366 3.37427

R13 3.25302 -0.00016 0.00020 0.00747 0.00767 3.26069

R14 3.47400 -0.00044 -0.00027 0.01166 0.01138 3.48538

R15 2.88186 -0.00030 -0.00095 0.00172 0.00077 2.88263

R16 2.06534 -0.00026 -0.00145 0.00284 0.00139 2.06673

R17 2.06132 -0.00044 -0.00138 0.00330 0.00193 2.06325

R18 2.89544 -0.00031 -0.00118 0.00074 -0.00045 2.89500

R19 2.07294 -0.00028 -0.00064 0.00234 0.00170 2.07464

R20 2.07208 -0.00030 -0.00109 0.00221 0.00112 2.07320

R21 2.88694 -0.00016 -0.00108 0.00183 0.00075 2.88769

R22 2.07288 -0.00037 -0.00100 0.00233 0.00132 2.07420

R23 2.07260 -0.00025 -0.00085 0.00161 0.00076 2.07336

R24 2.06828 -0.00026 -0.00079 0.00274 0.00195 2.07023

R25 2.07027 -0.00038 -0.00104 0.00211 0.00107 2.07134

R26 2.07001 -0.00031 -0.00105 0.00223 0.00118 2.07119

A1 2.17606 0.00039 0.00144 -0.00856 -0.00719 2.16887

A2 1.98154 -0.00113 -0.00506 0.00099 -0.00414 1.97739

A3 2.12514 0.00073 0.00376 0.00811 0.01179 2.13693

A4 2.02959 -0.00035 -0.00583 0.00108 -0.00475 2.02484

A5 1.82846 0.00035 0.00768 -0.03291 -0.02514 1.80331

A6 1.87689 0.00011 -0.00275 -0.01089 -0.01351 1.86338

A7 1.94367 0.00001 0.00153 0.01106 0.01235 1.95602

A8 1.93989 0.00015 -0.00087 -0.00009 -0.00131 1.93858

A9 1.83178 -0.00026 0.00116 0.03341 0.03436 1.86614

A10 1.87079 -0.00004 0.00300 0.01347 0.01647 1.88726

A11 1.91008 0.00037 0.00068 0.00656 0.00719 1.91727

A12 1.92832 0.00004 0.00004 -0.00808 -0.00803 1.92030

A13 1.95025 0.00016 0.00179 0.00831 0.01005 1.96031

A14 1.88720 -0.00028 -0.00254 -0.00048 -0.00300 1.88420

A15 1.89310 -0.00018 0.00069 0.00189 0.00248 1.89558

A16 1.89347 -0.00013 -0.00080 -0.00839 -0.00917 1.88430

A17 1.79834 -0.00069 -0.00229 0.02290 0.02061 1.81895

A18 1.96872 -0.00006 -0.00064 0.02568 0.02520 1.99392

A19 2.14114 0.00032 0.00065 -0.00061 0.00020 2.14134

A20 2.15959 -0.00028 -0.00375 -0.02167 -0.02527 2.13432

A21 1.79555 0.00013 0.00121 -0.00494 -0.00373 1.79181

A22 1.93027 -0.00063 -0.00409 0.00075 -0.00334 1.92692

A23 1.88005 0.00017 -0.00349 0.00132 -0.00217 1.87788

A24 1.88928 0.00023 0.00457 -0.00207 0.00249 1.89177

A25 1.93865 0.00005 0.00106 0.00412 0.00519 1.94384

A26 1.93839 0.00019 0.00066 -0.00593 -0.00527 1.93313

A27 1.88518 0.00000 0.00137 0.00190 0.00328 1.88845

A28 1.95113 0.00026 0.00237 0.00477 0.00713 1.95827

A29 1.91603 0.00005 0.00113 -0.00566 -0.00452 1.91150

A30 1.91851 -0.00023 -0.00274 0.00290 0.00013 1.91863

A31 1.90752 -0.00013 -0.00069 -0.00131 -0.00198 1.90554

A32 1.90754 0.00003 0.00126 0.00088 0.00212 1.90966

A33 1.86088 0.00001 -0.00152 -0.00189 -0.00342 1.85746

A34 1.96775 -0.00039 -0.00113 -0.00098 -0.00211 1.96564

A35 1.90545 0.00017 0.00038 0.00400 0.00438 1.90983

A36 1.90571 0.00019 0.00204 -0.00147 0.00057 1.90628

A37 1.91363 0.00002 -0.00070 0.00016 -0.00053 1.91310

A38 1.91172 0.00016 0.00078 0.00127 0.00205 1.91377

A39 1.85623 -0.00013 -0.00138 -0.00312 -0.00450 1.85173

A40 1.94440 0.00014 0.00095 0.00504 0.00598 1.95038

A41 1.94027 0.00022 0.00140 0.00375 0.00514 1.94541

A42 1.94327 -0.00015 0.00047 -0.00302 -0.00254 1.94073

A43 1.87841 -0.00016 -0.00146 -0.00359 -0.00508 1.87333

A44 1.87869 -0.00008 -0.00117 -0.00479 -0.00595 1.87273

A45 1.87558 0.00001 -0.00037 0.00225 0.00188 1.87746

D1 2.79031 -0.00005 -0.10037 0.07385 -0.02654 2.76377

D2 -1.33930 0.00000 -0.09628 0.06360 -0.03261 -1.37191

D3 0.60311 -0.00009 -0.09270 0.08221 -0.01040 0.59271

D4 -0.38325 -0.00026 -0.08814 0.09331 0.00506 -0.37819

D5 1.77033 -0.00020 -0.08405 0.08305 -0.00102 1.76931

D6 -2.57044 -0.00030 -0.08046 0.10166 0.02119 -2.54925

D7 -3.10236 0.00008 -0.00875 -0.00835 -0.01726 -3.11962

D8 0.00832 -0.00013 0.00302 0.01012 0.01329 0.02161

D9 -3.11191 0.00004 -0.00199 -0.07201 -0.07401 3.09726

D10 -1.03580 -0.00005 -0.00468 -0.07344 -0.07816 -1.11396

D11 1.07414 -0.00009 -0.00446 -0.08407 -0.08860 0.98554

D12 1.07872 -0.00018 -0.00918 -0.03764 -0.04674 1.03198

D13 -3.12835 -0.00027 -0.01186 -0.03907 -0.05089 3.10394

D14 -1.01841 -0.00031 -0.01164 -0.04970 -0.06133 -1.07974

D15 -0.95704 0.00005 -0.01104 -0.08612 -0.09712 -1.05416

D16 1.11907 -0.00004 -0.01372 -0.08756 -0.10127 1.01780

D17 -3.05417 -0.00008 -0.01350 -0.09818 -0.11172 3.11730

D18 -3.12898 0.00052 0.00962 0.12462 0.13409 -2.99488

D19 -0.92109 0.00034 0.00860 0.11035 0.11868 -0.80241

D20 1.17960 0.00036 0.00909 0.13658 0.14610 1.32570

D21 1.81740 0.00011 0.01301 0.03852 0.05154 1.86894

D22 -1.15282 0.00025 0.03360 0.01952 0.05310 -1.09972

D23 2.60785 -0.00001 -0.01758 -0.05771 -0.07526 2.53260

D24 -0.70721 -0.00009 -0.03791 -0.03600 -0.07394 -0.78116

D25 -3.05295 0.00028 0.00016 -0.12726 -0.12710 3.10313

D26 -0.93135 0.00007 -0.00324 -0.12090 -0.12414 -1.05549

D27 1.10303 0.00028 -0.00109 -0.11906 -0.12014 0.98289

D28 -3.12219 -0.00007 0.00683 0.01874 0.02557 -3.09663

D29 -1.00230 -0.00002 0.00832 0.01636 0.02467 -0.97762

D30 1.03936 -0.00011 0.00553 0.01243 0.01795 1.05731

D31 1.07436 0.00010 0.01321 0.01391 0.02712 1.10148

D32 -3.08893 0.00014 0.01470 0.01153 0.02623 -3.06271

D33 -1.04728 0.00005 0.01191 0.00760 0.01950 -1.02777

D34 -1.02413 -0.00007 0.01031 0.01273 0.02305 -1.00108

D35 1.09577 -0.00002 0.01180 0.01035 0.02215 1.11792

D36 3.13743 -0.00011 0.00901 0.00642 0.01543 -3.13033

D37 3.11796 0.00027 0.02752 0.03344 0.06096 -3.10426

D38 -1.03385 0.00015 0.02615 0.03585 0.06199 -0.97186

D39 0.98884 0.00020 0.02584 0.03353 0.05936 1.04820

D40 0.99316 0.00013 0.02500 0.03835 0.06334 1.05651

D41 3.12454 0.00001 0.02362 0.04075 0.06437 -3.09428

D42 -1.13596 0.00005 0.02331 0.03843 0.06174 -1.07422

D43 -1.03728 0.00017 0.02650 0.04086 0.06737 -0.96991

D44 1.09410 0.00005 0.02512 0.04327 0.06840 1.16249

D45 3.11678 0.00009 0.02481 0.04095 0.06577 -3.10064

D46 3.11856 -0.00004 0.00906 0.05416 0.06321 -3.10142

D47 -1.06958 0.00000 0.00879 0.05553 0.06433 -1.00525

D48 1.02113 0.00007 0.00958 0.05887 0.06845 1.08958

D49 0.99180 0.00000 0.00983 0.04958 0.05941 1.05121

D50 3.08685 0.00004 0.00957 0.05096 0.06053 -3.13581

D51 -1.10563 0.00011 0.01036 0.05430 0.06465 -1.04098

D52 -1.03889 0.00005 0.01145 0.05252 0.06396 -0.97493

D53 1.05615 0.00009 0.01118 0.05390 0.06508 1.12123

D54 -3.13633 0.00015 0.01197 0.05724 0.06921 -3.06712

Item Value Threshold Converged?

Maximum Force 0.004866 0.000450 NO

RMS Force 0.000517 0.000300 NO

Maximum Displacement 0.515261 0.001800 NO

RMS Displacement 0.100932 0.001200 NO

Predicted change in Energy=-1.516273D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:39:19 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.091452 -0.439757 -0.236030

2 6 0 -2.882017 0.101770 0.492142

3 8 0 -4.857388 0.237391 -0.880228

4 8 0 -4.243627 -1.780211 -0.099908

5 6 0 -2.349604 -0.753461 1.623622

6 16 0 -1.595051 0.330969 -0.901570

7 6 0 -0.108013 0.722347 -0.055132

8 16 0 1.096729 -0.595507 -0.041891

9 16 0 0.070741 2.144248 0.905878

10 6 0 2.696149 0.317829 -0.138958

11 6 0 3.868913 -0.656105 -0.084311

12 6 0 5.220812 0.064373 -0.098458

13 6 0 6.402964 -0.903924 -0.096629

14 1 0 -3.147718 1.097662 0.845378

15 1 0 -5.026227 -2.049327 -0.610492

16 1 0 -1.455844 -0.293448 2.046621

17 1 0 -3.098477 -0.831182 2.419585

18 1 0 -2.099622 -1.764267 1.296847

19 1 0 2.694964 0.888329 -1.072038

20 1 0 2.740534 1.024070 0.692505

21 1 0 3.795720 -1.267834 0.824376

22 1 0 3.817350 -1.351434 -0.931343

23 1 0 5.278643 0.714735 -0.980757

24 1 0 5.285789 0.727626 0.773130

25 1 0 7.361456 -0.374293 -0.065955

26 1 0 6.371805 -1.573281 0.770805

27 1 0 6.404632 -1.528955 -0.996967

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.512025 0.000000

3 O 1.208378 2.409126 0.000000

4 O 1.355914 2.397156 2.248626 0.000000

5 C 2.567246 1.514968 3.679679 2.759002 0.000000

6 S 2.696105 1.910823 3.263749 3.480617 2.849901

7 C 4.153432 2.894774 4.844846 4.834056 3.165589

8 S 5.194148 4.074531 6.070258 5.470492 3.830939

9 S 5.030396 3.614093 5.577879 5.918340 3.843168

10 C 6.830438 5.617909 7.590249 7.250088 5.451053

11 C 7.964749 6.817750 8.807959 8.190064 6.449532

12 C 9.326915 8.124410 10.109957 9.642515 7.806767

13 C 10.505602 9.357828 11.345139 10.682593 8.921287

14 H 2.103268 1.089575 2.576967 3.221294 2.160858

15 H 1.898616 3.231201 2.308754 0.972412 3.719523

16 H 3.489747 2.146292 4.518711 3.819657 1.090572

17 H 2.862080 2.152275 3.889008 2.925725 1.095631

18 H 2.841026 2.177564 4.043707 2.558893 1.091331

19 H 6.965498 5.845344 7.582779 7.497344 5.950607

20 H 7.048475 5.701216 7.798768 7.567721 5.471389

21 H 8.001104 6.824834 8.946936 8.108510 6.218391

22 H 7.991481 7.001401 8.819187 8.115077 6.701995

23 H 9.470278 8.315139 10.147764 9.883030 8.193202

24 H 9.503359 8.196566 10.288730 9.892482 7.824077

25 H 11.454358 10.269704 12.261213 11.689983 9.864234

26 H 10.572528 9.408330 11.493443 10.653091 8.801272

27 H 10.579847 9.545603 11.400294 10.688931 9.170906

6 7 8 9 10

6 S 0.000000

7 C 1.755254 0.000000

8 S 2.973733 1.785586 0.000000

9 S 3.054457 1.725484 3.075252 0.000000

10 C 4.358457 2.834429 1.844383 3.364559 0.000000

11 C 5.612230 4.209147 2.773171 4.821676 1.525421

12 C 6.868192 5.369468 4.176926 5.644272 2.537677

13 C 8.132721 6.711133 5.315473 7.098833 3.903198

14 H 2.459760 3.192426 4.655039 3.384889 5.977276

15 H 4.186109 5.672692 6.318820 6.772336 8.090789

16 H 3.016804 2.695525 3.311910 3.094207 4.731750

17 H 3.826350 4.180974 4.869718 4.603089 6.437706

18 H 3.078579 3.460867 3.657168 4.487741 5.421815

19 H 4.329427 2.986357 2.411914 3.517958 1.093668

20 H 4.671056 2.960442 2.421665 2.903123 1.091823

21 H 5.881792 4.469171 2.913245 5.052169 2.156710

22 H 5.667932 4.525128 2.960461 5.443551 2.161343

23 H 6.884855 5.465611 4.481809 5.720590 2.745075

24 H 7.092807 5.457027 4.468016 5.405660 2.775981

25 H 9.023007 7.549549 6.268678 7.774447 4.716932

26 H 8.360252 6.923881 5.426136 7.317218 4.232543

27 H 8.213607 6.954851 5.473329 7.565144 4.230796

11 12 13 14 15

11 C 0.000000

12 C 1.531967 0.000000

13 C 2.546171 1.528098 0.000000

14 H 7.291990 8.484740 9.803533 0.000000

15 H 9.018949 10.475291 11.497931 3.943590 0.000000

16 H 5.746775 7.021904 8.168664 2.498121 4.784454

17 H 7.405718 8.738028 9.829243 2.490179 3.792291

18 H 6.225675 7.673302 8.658865 3.081066 3.504886

19 H 2.176933 2.829607 4.232359 6.152823 8.274034

20 H 2.167872 2.774603 4.213465 5.890696 8.453766

21 H 1.097853 2.158074 2.788979 7.335349 8.971975

22 H 1.097088 2.160535 2.753618 7.593877 8.876872

23 H 2.161055 1.097619 2.160055 8.630467 10.675556

24 H 2.158114 1.097174 2.160212 8.441929 10.768637

25 H 3.503942 2.185369 1.095516 10.650817 12.512272

26 H 2.799448 2.182272 1.096108 9.887407 11.491290

27 H 2.832786 2.178862 1.096027 10.076742 11.449222

16 17 18 19 20

16 H 0.000000

17 H 1.768192 0.000000

18 H 1.771982 1.768869 0.000000

19 H 5.324644 6.979405 5.969584 0.000000

20 H 4.602073 6.365439 5.618466 1.770343 0.000000

21 H 5.479255 7.089803 5.935043 3.075238 2.526585

22 H 6.147697 7.702470 6.336073 2.509200 3.072366

23 H 7.452166 9.172149 8.109977 2.591113 3.055731

24 H 6.936424 8.685425 7.812048 3.184783 2.563728

25 H 9.067209 10.760894 9.659257 4.937870 4.887084

26 H 8.033541 9.641340 8.489893 4.793199 4.465254

27 H 8.519212 10.122686 8.811316 4.428379 4.774711

21 22 23 24 25

21 H 0.000000

22 H 1.757841 0.000000

23 H 3.064008 2.531180 0.000000

24 H 2.490941 3.063336 1.753949 0.000000

25 H 3.782271 3.776822 2.522093 2.495332 0.000000

26 H 2.594684 3.077623 3.081881 2.544329 1.765545

27 H 3.192474 2.594195 2.510430 3.078508 1.765090

26 27

26 H 0.000000

27 H 1.768631 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 2.00D-01

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.109075 -0.483615 -0.150735

2 6 0 -2.893662 0.199557 0.434302

3 8 0 -4.875702 0.037984 -0.925586

4 8 0 -4.265862 -1.759890 0.279429

5 6 0 -2.358686 -0.386652 1.724763

6 16 0 -1.613177 0.108034 -0.981052

7 6 0 -0.120140 0.669562 -0.248629

8 16 0 1.079399 -0.618732 0.050904

9 16 0 0.069348 2.268006 0.372957

10 6 0 2.681907 0.242363 -0.252795

11 6 0 3.851057 -0.701222 0.011110

12 6 0 5.205720 -0.008591 -0.167971

13 6 0 6.384001 -0.958417 0.043139

14 1 0 -3.153526 1.250267 0.559418

15 1 0 -5.052215 -2.131403 -0.155555

16 1 0 -1.460879 0.151066 2.031598

17 1 0 -3.103646 -0.282455 2.521371

18 1 0 -2.114460 -1.445969 1.628821

19 1 0 2.678062 0.592147 -1.289012

20 1 0 2.733497 1.114912 0.401478

21 1 0 3.780232 -1.096235 1.032986

22 1 0 3.792251 -1.566539 -0.660731

23 1 0 5.261477 0.430017 -1.172602

24 1 0 5.277941 0.830817 0.534860

25 1 0 7.344742 -0.439985 -0.048301

26 1 0 6.354762 -1.418974 1.037364

27 1 0 6.378423 -1.767253 -0.696475

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3136405 0.1917705 0.1805220

Leave Link 202 at Sat Aug 17 17:39:19 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1100.7998697317 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0548057612 Hartrees.

Nuclear repulsion after empirical dispersion term = 1100.7450639704 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2307

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.76D-09

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 84

GePol: Fraction of low-weight points (<1% of avg) = 3.64%

GePol: Cavity surface area = 309.807 Ang\*\*2

GePol: Cavity volume = 321.065 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0056604227 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1100.7394035477 Hartrees.

Leave Link 301 at Sat Aug 17 17:39:19 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.87D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:39:19 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:39:19 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999080 0.042890 0.000732 0.000026 Ang= 4.92 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.62829414036

Leave Link 401 at Sat Aug 17 17:39:20 2019, MaxMem= 1342177280 cpu: 7.5

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 15966747.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.22D-15 for 2270.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.68D-15 for 744 103.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.00D-15 for 577.

Iteration 1 A^-1\*A deviation from orthogonality is 4.30D-12 for 600 580.

E= -1658.65182425667

DIIS: error= 4.92D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.65182425667 IErMin= 1 ErrMin= 4.92D-03

ErrMax= 4.92D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.67D-02 BMatP= 5.67D-02

IDIUse=3 WtCom= 9.51D-01 WtEn= 4.92D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.429 Goal= None Shift= 0.000

Gap= 0.483 Goal= None Shift= 0.000

GapD= 0.429 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=5.52D-04 MaxDP=1.22D-02 OVMax= 2.81D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 5.51D-04 CP: 9.99D-01

E= -1658.67584238409 Delta-E= -0.024018127418 Rises=F Damp=F

DIIS: error= 9.35D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67584238409 IErMin= 2 ErrMin= 9.35D-04

ErrMax= 9.35D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.02D-03 BMatP= 5.67D-02

IDIUse=3 WtCom= 9.91D-01 WtEn= 9.35D-03

Coeff-Com: -0.507D-01 0.105D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.502D-01 0.105D+01

Gap= 0.124 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=1.02D-04 MaxDP=3.21D-03 DE=-2.40D-02 OVMax= 6.94D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 9.16D-05 CP: 9.99D-01 1.08D+00

E= -1658.67590655239 Delta-E= -0.000064168294 Rises=F Damp=F

DIIS: error= 1.88D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67590655239 IErMin= 2 ErrMin= 9.35D-04

ErrMax= 1.88D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.58D-03 BMatP= 1.02D-03

IDIUse=3 WtCom= 1.87D-01 WtEn= 8.13D-01

Coeff-Com: -0.413D-01 0.617D+00 0.424D+00

Coeff-En: 0.000D+00 0.419D+00 0.581D+00

Coeff: -0.773D-02 0.457D+00 0.551D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=6.90D-05 MaxDP=3.22D-03 DE=-6.42D-05 OVMax= 7.66D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 4.80D-05 CP: 9.98D-01 1.10D+00 4.75D-01

E= -1658.67606579330 Delta-E= -0.000159240914 Rises=F Damp=F

DIIS: error= 1.41D-03 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67606579330 IErMin= 2 ErrMin= 9.35D-04

ErrMax= 1.41D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.39D-04 BMatP= 1.02D-03

IDIUse=3 WtCom= 9.86D-01 WtEn= 1.41D-02

Coeff-Com: -0.142D-01 0.176D+00 0.394D+00 0.445D+00

Coeff-En: 0.000D+00 0.000D+00 0.346D+00 0.654D+00

Coeff: -0.140D-01 0.173D+00 0.393D+00 0.448D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=2.99D-05 MaxDP=1.17D-03 DE=-1.59D-04 OVMax= 3.62D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.38D-05 CP: 9.98D-01 1.11D+00 6.82D-01 6.15D-01

E= -1658.67619450856 Delta-E= -0.000128715263 Rises=F Damp=F

DIIS: error= 1.15D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67619450856 IErMin= 5 ErrMin= 1.15D-04

ErrMax= 1.15D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.71D-05 BMatP= 7.39D-04

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.15D-03

Coeff-Com: -0.408D-02 0.393D-01 0.188D+00 0.263D+00 0.514D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.407D-02 0.392D-01 0.188D+00 0.262D+00 0.514D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=5.57D-06 MaxDP=3.17D-04 DE=-1.29D-04 OVMax= 4.00D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 4.23D-06 CP: 9.98D-01 1.11D+00 6.99D-01 6.70D-01 8.82D-01

E= -1658.67619774911 Delta-E= -0.000003240551 Rises=F Damp=F

DIIS: error= 3.13D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67619774911 IErMin= 6 ErrMin= 3.13D-05

ErrMax= 3.13D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.03D-06 BMatP= 1.71D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.493D-03-0.128D-01 0.187D-01 0.441D-01 0.220D+00 0.730D+00

Coeff: 0.493D-03-0.128D-01 0.187D-01 0.441D-01 0.220D+00 0.730D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=2.80D-06 MaxDP=1.20D-04 DE=-3.24D-06 OVMax= 3.09D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.85D-06 CP: 9.98D-01 1.11D+00 7.16D-01 6.92D-01 9.36D-01

CP: 9.56D-01

E= -1658.67619801545 Delta-E= -0.000000266338 Rises=F Damp=F

DIIS: error= 9.63D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67619801545 IErMin= 7 ErrMin= 9.63D-06

ErrMax= 9.63D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.53D-07 BMatP= 1.03D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.634D-03-0.989D-02-0.106D-01-0.603D-02 0.458D-01 0.333D+00

Coeff-Com: 0.647D+00

Coeff: 0.634D-03-0.989D-02-0.106D-01-0.603D-02 0.458D-01 0.333D+00

Coeff: 0.647D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=1.19D-06 MaxDP=4.96D-05 DE=-2.66D-07 OVMax= 1.33D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 8.15D-07 CP: 9.98D-01 1.11D+00 7.17D-01 7.03D-01 9.73D-01

CP: 1.05D+00 1.02D+00

E= -1658.67619806304 Delta-E= -0.000000047588 Rises=F Damp=F

DIIS: error= 3.99D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67619806304 IErMin= 8 ErrMin= 3.99D-06

ErrMax= 3.99D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.54D-08 BMatP= 1.53D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.165D-03-0.150D-02-0.813D-02-0.112D-01-0.240D-01-0.498D-02

Coeff-Com: 0.281D+00 0.768D+00

Coeff: 0.165D-03-0.150D-02-0.813D-02-0.112D-01-0.240D-01-0.498D-02

Coeff: 0.281D+00 0.768D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=6.01D-07 MaxDP=2.96D-05 DE=-4.76D-08 OVMax= 5.61D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.93D-07 CP: 9.98D-01 1.11D+00 7.19D-01 7.06D-01 9.89D-01

CP: 1.11D+00 1.20D+00 9.61D-01

E= -1658.67619807338 Delta-E= -0.000000010340 Rises=F Damp=F

DIIS: error= 1.77D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67619807338 IErMin= 9 ErrMin= 1.77D-06

ErrMax= 1.77D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.46D-09 BMatP= 2.54D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.297D-04 0.975D-03-0.162D-02-0.369D-02-0.168D-01-0.531D-01

Coeff-Com: 0.919D-02 0.305D+00 0.760D+00

Coeff: -0.297D-04 0.975D-03-0.162D-02-0.369D-02-0.168D-01-0.531D-01

Coeff: 0.919D-02 0.305D+00 0.760D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=2.52D-07 MaxDP=1.05D-05 DE=-1.03D-08 OVMax= 3.12D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.19D-07 CP: 9.98D-01 1.11D+00 7.19D-01 7.07D-01 9.92D-01

CP: 1.13D+00 1.27D+00 1.11D+00 8.81D-01

E= -1658.67619807475 Delta-E= -0.000000001370 Rises=F Damp=F

DIIS: error= 8.66D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67619807475 IErMin=10 ErrMin= 8.66D-07

ErrMax= 8.66D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.25D-10 BMatP= 3.46D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.361D-04 0.689D-03 0.193D-03-0.526D-03-0.539D-02-0.267D-01

Coeff-Com: -0.335D-01 0.494D-01 0.376D+00 0.640D+00

Coeff: -0.361D-04 0.689D-03 0.193D-03-0.526D-03-0.539D-02-0.267D-01

Coeff: -0.335D-01 0.494D-01 0.376D+00 0.640D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=7.45D-08 MaxDP=2.96D-06 DE=-1.37D-09 OVMax= 6.64D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 4.31D-08 CP: 9.98D-01 1.11D+00 7.20D-01 7.08D-01 9.92D-01

CP: 1.13D+00 1.29D+00 1.14D+00 1.01D+00 8.17D-01

E= -1658.67619807495 Delta-E= -0.000000000198 Rises=F Damp=F

DIIS: error= 2.20D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67619807495 IErMin=11 ErrMin= 2.20D-07

ErrMax= 2.20D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.44D-11 BMatP= 7.25D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.946D-05 0.127D-03 0.257D-03 0.240D-03 0.162D-03-0.275D-02

Coeff-Com: -0.134D-01-0.173D-01 0.513D-01 0.239D+00 0.742D+00

Coeff: -0.946D-05 0.127D-03 0.257D-03 0.240D-03 0.162D-03-0.275D-02

Coeff: -0.134D-01-0.173D-01 0.513D-01 0.239D+00 0.742D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=2.89D-08 MaxDP=1.17D-06 DE=-1.98D-10 OVMax= 3.23D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.99D-08 CP: 9.98D-01 1.11D+00 7.20D-01 7.07D-01 9.92D-01

CP: 1.13D+00 1.29D+00 1.15D+00 1.03D+00 9.53D-01

CP: 9.39D-01

E= -1658.67619807495 Delta-E= -0.000000000007 Rises=F Damp=F

DIIS: error= 1.37D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.67619807495 IErMin=12 ErrMin= 1.37D-07

ErrMax= 1.37D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.73D-11 BMatP= 6.44D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.125D-05-0.624D-04 0.136D-03 0.284D-03 0.129D-02 0.392D-02

Coeff-Com: -0.187D-02-0.232D-01-0.491D-01 0.230D-01 0.495D+00 0.550D+00

Coeff: 0.125D-05-0.624D-04 0.136D-03 0.284D-03 0.129D-02 0.392D-02

Coeff: -0.187D-02-0.232D-01-0.491D-01 0.230D-01 0.495D+00 0.550D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=1.32D-08 MaxDP=7.98D-07 DE=-7.28D-12 OVMax= 1.56D-06

Cycle 13 Pass 1 IDiag 1:

RMSU= 8.68D-09 CP: 9.98D-01 1.11D+00 7.20D-01 7.07D-01 9.92D-01

CP: 1.13D+00 1.29D+00 1.15D+00 1.04D+00 9.67D-01

CP: 1.08D+00 6.94D-01

E= -1658.67619807496 Delta-E= -0.000000000005 Rises=F Damp=F

DIIS: error= 4.24D-08 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1658.67619807496 IErMin=13 ErrMin= 4.24D-08

ErrMax= 4.24D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.68D-12 BMatP= 3.73D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.265D-05-0.583D-04 0.150D-04 0.979D-04 0.621D-03 0.259D-02

Coeff-Com: 0.217D-02-0.750D-02-0.357D-01-0.436D-01 0.840D-01 0.290D+00

Coeff-Com: 0.707D+00

Coeff: 0.265D-05-0.583D-04 0.150D-04 0.979D-04 0.621D-03 0.259D-02

Coeff: 0.217D-02-0.750D-02-0.357D-01-0.436D-01 0.840D-01 0.290D+00

Coeff: 0.707D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=6.92D-09 MaxDP=2.66D-07 DE=-4.55D-12 OVMax= 6.13D-07

Error on total polarization charges = 0.04183

SCF Done: E(UB3LYP) = -1658.67619807 A.U. after 13 cycles

NFock= 13 Conv=0.69D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7553 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655183513420D+03 PE=-6.144238536499D+03 EE= 1.729639421456D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.55

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7553, after 0.7500

Leave Link 502 at Sat Aug 17 17:39:47 2019, MaxMem= 1342177280 cpu: 313.0

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 335

Leave Link 701 at Sat Aug 17 17:39:48 2019, MaxMem= 1342177280 cpu: 10.2

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:39:48 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:39:51 2019, MaxMem= 1342177280 cpu: 36.0

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.25360847D+00-2.85220085D+00 6.49616427D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.001661159 -0.002666159 0.008294207

2 6 -0.003200095 -0.004263942 -0.003703905

3 8 -0.001340713 0.000448070 -0.003364004

4 8 0.001606515 0.003100159 -0.001294290

5 6 -0.000441991 -0.001301669 0.000913723

6 16 0.001128190 0.000575148 0.000618173

7 6 -0.001055541 0.003143363 0.002329499

8 16 0.001706059 -0.001566658 -0.000056162

9 16 -0.001408070 0.000528175 -0.000759795

10 6 0.000072327 -0.000325489 -0.000141876

11 6 -0.000658787 -0.001161785 -0.000140328

12 6 0.000091322 0.000979864 0.000017181

13 6 0.001073414 -0.000710811 -0.000235124

14 1 0.001724377 0.000666012 -0.001242397

15 1 0.000281330 0.001506985 -0.000145369

16 1 0.000166358 0.000200061 -0.000046564

17 1 0.000531468 0.000183182 -0.000193392

18 1 0.000176454 0.000990529 -0.000539160

19 1 0.000500770 -0.000146150 0.000703441

20 1 -0.001194927 -0.000945728 -0.000792159

21 1 0.000225300 0.000584960 -0.000682012

22 1 0.000147753 0.000404819 0.000318647

23 1 0.000066117 -0.000687441 0.000391970

24 1 -0.000210156 -0.000427658 -0.000319118

25 1 -0.001006284 0.000158197 -0.000103747

26 1 -0.000375823 0.000550345 -0.000556890

27 1 -0.000266525 0.000183621 0.000729452

-------------------------------------------------------------------

Cartesian Forces: Max 0.008294207 RMS 0.001568433

Leave Link 716 at Sat Aug 17 17:39:51 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.004904951 RMS 0.001146206

Search for a local minimum.

Step number 22 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .11462D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 19

DE= 7.76D-04 DEPred=-1.52D-04 R=-5.12D+00

Trust test=-5.12D+00 RLast= 5.64D-01 DXMaxT set to 5.95D-02

ITU= -1 1 -1 1 -1 1 1 -1 1 -1 1 1 -1 0 0 -1 0 0 -1 -1

ITU= 0 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.93634.

Iteration 1 RMS(Cart)= 0.09446503 RMS(Int)= 0.00444339

Iteration 2 RMS(Cart)= 0.00840810 RMS(Int)= 0.00001689

Iteration 3 RMS(Cart)= 0.00005825 RMS(Int)= 0.00000431

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000431

ITry= 1 IFail=0 DXMaxC= 4.54D-01 DCOld= 1.00D+10 DXMaxT= 5.95D-02 DXLimC= 3.00D+00 Rises=T

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.85731 -0.00431 -0.01842 0.00000 -0.01842 2.83889

R2 2.28350 0.00289 0.00441 0.00000 0.00441 2.28791

R3 2.56231 -0.00490 -0.00847 0.00000 -0.00847 2.55384

R4 2.86288 0.00024 0.00354 0.00000 0.00354 2.86642

R5 3.61093 -0.00157 -0.01312 0.00000 -0.01312 3.59781

R6 2.05900 -0.00022 -0.00081 0.00000 -0.00081 2.05818

R7 1.83759 -0.00057 -0.00052 0.00000 -0.00052 1.83707

R8 2.06088 0.00020 0.00056 0.00000 0.00056 2.06144

R9 2.07044 -0.00052 -0.00153 0.00000 -0.00153 2.06891

R10 2.06232 -0.00071 -0.00182 0.00000 -0.00182 2.06049

R11 3.31695 -0.00151 0.00321 0.00000 0.00321 3.32016

R12 3.37427 0.00237 0.00904 0.00000 0.00904 3.38331

R13 3.26069 -0.00013 -0.00609 0.00000 -0.00609 3.25460

R14 3.48538 -0.00203 -0.00834 0.00000 -0.00834 3.47704

R15 2.88263 -0.00067 -0.00150 0.00000 -0.00150 2.88113

R16 2.06673 -0.00068 -0.00274 0.00000 -0.00274 2.06399

R17 2.06325 -0.00126 -0.00272 0.00000 -0.00272 2.06053

R18 2.89500 -0.00052 -0.00062 0.00000 -0.00062 2.89437

R19 2.07464 -0.00091 -0.00209 0.00000 -0.00209 2.07255

R20 2.07320 -0.00051 -0.00210 0.00000 -0.00210 2.07110

R21 2.88769 -0.00057 -0.00163 0.00000 -0.00163 2.88606

R22 2.07420 -0.00071 -0.00200 0.00000 -0.00200 2.07220

R23 2.07336 -0.00053 -0.00148 0.00000 -0.00148 2.07188

R24 2.07023 -0.00080 -0.00233 0.00000 -0.00233 2.06790

R25 2.07134 -0.00078 -0.00195 0.00000 -0.00195 2.06940

R26 2.07119 -0.00070 -0.00197 0.00000 -0.00197 2.06922

A1 2.16887 0.00128 0.00777 0.00000 0.00778 2.17664

A2 1.97739 -0.00007 -0.00124 0.00000 -0.00123 1.97616

A3 2.13693 -0.00121 -0.00703 0.00000 -0.00702 2.12991

A4 2.02484 -0.00013 -0.00141 0.00000 -0.00141 2.02344

A5 1.80331 0.00135 0.03207 0.00000 0.03207 1.83538

A6 1.86338 0.00001 0.00744 0.00000 0.00743 1.87081

A7 1.95602 -0.00093 -0.00891 0.00000 -0.00889 1.94712

A8 1.93858 0.00074 0.00135 0.00000 0.00136 1.93995

A9 1.86614 -0.00108 -0.03168 0.00000 -0.03167 1.83447

A10 1.88726 -0.00262 -0.01301 0.00000 -0.01301 1.87425

A11 1.91727 -0.00021 -0.00535 0.00000 -0.00535 1.91191

A12 1.92030 0.00051 0.00774 0.00000 0.00774 1.92804

A13 1.96031 -0.00098 -0.00744 0.00000 -0.00744 1.95287

A14 1.88420 -0.00007 -0.00039 0.00000 -0.00039 1.88381

A15 1.89558 0.00029 -0.00212 0.00000 -0.00212 1.89346

A16 1.88430 0.00050 0.00781 0.00000 0.00781 1.89211

A17 1.81895 -0.00311 -0.02423 0.00000 -0.02423 1.79471

A18 1.99392 -0.00425 -0.02022 0.00000 -0.02021 1.97371

A19 2.14134 -0.00046 0.00055 0.00000 0.00055 2.14189

A20 2.13432 0.00469 0.01832 0.00000 0.01832 2.15265

A21 1.79181 0.00138 0.00095 0.00000 0.00095 1.79276

A22 1.92692 0.00003 0.00167 0.00000 0.00167 1.92859

A23 1.87788 0.00047 -0.00318 0.00000 -0.00318 1.87470

A24 1.89177 -0.00093 0.00325 0.00000 0.00326 1.89503

A25 1.94384 -0.00055 -0.00496 0.00000 -0.00496 1.93888

A26 1.93313 0.00105 0.00491 0.00000 0.00491 1.93804

A27 1.88845 -0.00011 -0.00182 0.00000 -0.00182 1.88663

A28 1.95827 -0.00078 -0.00553 0.00000 -0.00553 1.95273

A29 1.91150 0.00021 0.00615 0.00000 0.00615 1.91765

A30 1.91863 0.00038 -0.00319 0.00000 -0.00319 1.91544

A31 1.90554 0.00026 0.00041 0.00000 0.00041 1.90595

A32 1.90966 0.00003 0.00051 0.00000 0.00051 1.91017

A33 1.85746 -0.00006 0.00207 0.00000 0.00207 1.85953

A34 1.96564 -0.00001 0.00158 0.00000 0.00158 1.96722

A35 1.90983 -0.00003 -0.00324 0.00000 -0.00324 1.90659

A36 1.90628 -0.00005 0.00050 0.00000 0.00050 1.90678

A37 1.91310 -0.00007 -0.00033 0.00000 -0.00033 1.91277

A38 1.91377 0.00005 -0.00093 0.00000 -0.00093 1.91284

A39 1.85173 0.00012 0.00247 0.00000 0.00247 1.85420

A40 1.95038 -0.00075 -0.00481 0.00000 -0.00481 1.94557

A41 1.94541 -0.00042 -0.00290 0.00000 -0.00290 1.94251

A42 1.94073 0.00011 0.00271 0.00000 0.00271 1.94344

A43 1.87333 0.00060 0.00292 0.00000 0.00292 1.87626

A44 1.87273 0.00043 0.00401 0.00000 0.00401 1.87675

A45 1.87746 0.00009 -0.00160 0.00000 -0.00160 1.87586

D1 2.76377 0.00131 -0.09037 0.00000 -0.09037 2.67340

D2 -1.37191 0.00105 -0.07852 0.00000 -0.07852 -1.45043

D3 0.59271 0.00042 -0.09713 0.00000 -0.09713 0.49558

D4 -0.37819 -0.00057 -0.12235 0.00000 -0.12234 -0.50053

D5 1.76931 -0.00082 -0.11049 0.00000 -0.11049 1.65882

D6 -2.54925 -0.00145 -0.12911 0.00000 -0.12911 -2.67836

D7 -3.11962 0.00096 0.01475 0.00000 0.01476 -3.10486

D8 0.02161 -0.00087 -0.01624 0.00000 -0.01624 0.00537

D9 3.09726 0.00004 0.06226 0.00000 0.06226 -3.12366

D10 -1.11396 0.00014 0.06320 0.00000 0.06320 -1.05076

D11 0.98554 0.00047 0.07349 0.00000 0.07349 1.05903

D12 1.03198 -0.00094 0.02754 0.00000 0.02754 1.05952

D13 3.10394 -0.00085 0.02849 0.00000 0.02849 3.13243

D14 -1.07974 -0.00051 0.03877 0.00000 0.03877 -1.04097

D15 -1.05416 0.00056 0.07235 0.00000 0.07235 -0.98182

D16 1.01780 0.00065 0.07329 0.00000 0.07329 1.09109

D17 3.11730 0.00098 0.08358 0.00000 0.08358 -3.08231

D18 -2.99488 -0.00037 -0.14715 0.00000 -0.14713 3.14117

D19 -0.80241 -0.00016 -0.13246 0.00000 -0.13245 -0.93487

D20 1.32570 -0.00054 -0.15625 0.00000 -0.15628 1.16942

D21 1.86894 -0.00109 -0.01997 0.00000 -0.01997 1.84896

D22 -1.09972 -0.00144 -0.01353 0.00000 -0.01353 -1.11325

D23 2.53260 -0.00085 0.01397 0.00000 0.01397 2.54657

D24 -0.78116 -0.00107 0.00548 0.00000 0.00548 -0.77568

D25 3.10313 0.00054 0.17910 0.00000 0.17910 -3.00095

D26 -1.05549 0.00019 0.17202 0.00000 0.17202 -0.88347

D27 0.98289 -0.00018 0.16988 0.00000 0.16988 1.15277

D28 -3.09663 0.00007 -0.00557 0.00000 -0.00557 -3.10219

D29 -0.97762 0.00003 -0.00448 0.00000 -0.00448 -0.98210

D30 1.05731 0.00030 -0.00024 0.00000 -0.00024 1.05707

D31 1.10148 -0.00019 0.00052 0.00000 0.00052 1.10199

D32 -3.06271 -0.00023 0.00161 0.00000 0.00161 -3.06110

D33 -1.02777 0.00005 0.00585 0.00000 0.00585 -1.02193

D34 -1.00108 -0.00039 0.00284 0.00000 0.00284 -0.99824

D35 1.11792 -0.00043 0.00393 0.00000 0.00393 1.12185

D36 -3.13033 -0.00016 0.00817 0.00000 0.00817 -3.12216

D37 -3.10426 -0.00005 -0.02035 0.00000 -0.02035 -3.12461

D38 -0.97186 -0.00017 -0.02202 0.00000 -0.02202 -0.99387

D39 1.04820 -0.00007 -0.02058 0.00000 -0.02058 1.02761

D40 1.05651 0.00002 -0.02476 0.00000 -0.02476 1.03175

D41 -3.09428 -0.00011 -0.02642 0.00000 -0.02642 -3.12070

D42 -1.07422 0.00000 -0.02499 0.00000 -0.02499 -1.09921

D43 -0.96991 -0.00007 -0.02775 0.00000 -0.02775 -0.99766

D44 1.16249 -0.00020 -0.02942 0.00000 -0.02942 1.13307

D45 -3.10064 -0.00009 -0.02799 0.00000 -0.02799 -3.12862

D46 -3.10142 -0.00004 -0.03489 0.00000 -0.03489 -3.13630

D47 -1.00525 -0.00007 -0.03642 0.00000 -0.03642 -1.04168

D48 1.08958 -0.00016 -0.03858 0.00000 -0.03858 1.05100

D49 1.05121 0.00006 -0.03158 0.00000 -0.03158 1.01963

D50 -3.13581 0.00003 -0.03311 0.00000 -0.03311 3.11426

D51 -1.04098 -0.00006 -0.03527 0.00000 -0.03527 -1.07625

D52 -0.97493 -0.00007 -0.03383 0.00000 -0.03383 -1.00876

D53 1.12123 -0.00010 -0.03537 0.00000 -0.03537 1.08586

D54 -3.06712 -0.00020 -0.03753 0.00000 -0.03753 -3.10465

Item Value Threshold Converged?

Maximum Force 0.004905 0.000450 NO

RMS Force 0.001146 0.000300 NO

Maximum Displacement 0.454437 0.001800 NO

RMS Displacement 0.095089 0.001200 NO

Predicted change in Energy=-2.009753D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:39:51 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.105496 -0.411853 -0.215898

2 6 0 -2.842952 0.055496 0.450735

3 8 0 -4.883347 0.308066 -0.801118

4 8 0 -4.285684 -1.748967 -0.138253

5 6 0 -2.352941 -0.790319 1.610606

6 16 0 -1.549183 0.148711 -0.942902

7 6 0 -0.108039 0.697925 -0.101265

8 16 0 1.108246 -0.596079 0.125944

9 16 0 -0.007265 2.236837 0.665401

10 6 0 2.700379 0.316179 -0.009652

11 6 0 3.872994 -0.657782 -0.038992

12 6 0 5.219017 0.070861 -0.095662

13 6 0 6.406693 -0.887763 -0.149661

14 1 0 -3.004269 1.087924 0.757826

15 1 0 -5.102292 -1.960581 -0.621386

16 1 0 -1.445915 -0.349289 2.026284

17 1 0 -3.105870 -0.824152 2.404703

18 1 0 -2.130746 -1.812516 1.302971

19 1 0 2.659798 0.910117 -0.925365

20 1 0 2.781338 1.001053 0.834937

21 1 0 3.847198 -1.299249 0.850228

22 1 0 3.780965 -1.322121 -0.905798

23 1 0 5.237177 0.728629 -0.972852

24 1 0 5.313419 0.724387 0.779593

25 1 0 7.357109 -0.346491 -0.184217

26 1 0 6.431234 -1.540538 0.729246

27 1 0 6.360593 -1.530123 -1.035230

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.502276 0.000000

3 O 1.210709 2.407102 0.000000

4 O 1.351432 2.384213 2.242315 0.000000

5 C 2.559454 1.516844 3.664126 2.777231 0.000000

6 S 2.716156 1.903878 3.340980 3.425942 2.836937

7 C 4.150230 2.863069 4.842039 4.841628 3.191388

8 S 5.228184 4.017711 6.129935 5.522086 3.771176

9 S 4.958603 3.584055 5.444906 5.902318 3.944525

10 C 6.847810 5.568521 7.624918 7.286044 5.420850

11 C 7.984240 6.771449 8.842353 8.231923 6.442127

12 C 9.337773 8.080478 10.129742 9.677444 7.809451

13 C 10.523165 9.316981 11.371869 10.727009 8.935280

14 H 2.100041 1.089144 2.563088 3.239280 2.163159

15 H 1.885890 3.212263 2.286264 0.972136 3.729643

16 H 3.479176 2.144275 4.499139 3.835180 1.090867

17 H 2.834924 2.158911 3.836487 2.951927 1.094823

18 H 2.858051 2.173249 4.062126 2.593245 1.090366

19 H 6.929657 5.736225 7.568152 7.478635 5.869428

20 H 7.108378 5.716146 7.867928 7.645424 5.492858

21 H 8.072760 6.837619 9.029553 8.205066 6.267289

22 H 7.968740 6.900310 8.816959 8.114317 6.651308

23 H 9.442416 8.232144 10.130714 9.875218 8.160353

24 H 9.539287 8.190356 10.326955 9.955033 7.858625

25 H 11.462835 10.227707 12.273458 11.727049 9.884505

26 H 10.639075 9.414638 11.566291 10.753991 8.860099

27 H 10.557503 9.456613 11.395610 10.686238 9.136380

6 7 8 9 10

6 S 0.000000

7 C 1.756953 0.000000

8 S 2.959573 1.790370 0.000000

9 S 3.053591 1.722260 3.092053 0.000000

10 C 4.354052 2.835725 1.839969 3.387618 0.000000

11 C 5.555851 4.206001 2.770350 4.891973 1.524627

12 C 6.821466 5.363839 4.170414 5.708300 2.532018

13 C 8.062225 6.705109 5.313622 7.180968 3.899467

14 H 2.427318 3.046027 4.488643 3.211008 5.807548

15 H 4.144523 5.681615 6.402434 6.725581 8.151045

16 H 3.012430 2.722689 3.193108 3.257263 4.666866

17 H 3.817879 4.193278 4.796200 4.690008 6.390773

18 H 3.037857 3.516467 3.654611 4.616593 5.440045

19 H 4.277331 2.895702 2.404411 3.376972 1.092218

20 H 4.758215 3.052354 2.419243 3.054867 1.090384

21 H 5.867950 4.531882 2.919057 5.234019 2.159675

22 H 5.529484 4.455583 2.955512 5.430058 2.157492

23 H 6.811159 5.415898 4.473285 5.697608 2.744671

24 H 7.098851 5.492615 4.455823 5.532650 2.759985

25 H 8.952254 7.538311 6.261532 7.850442 4.706883

26 H 8.326866 6.961506 5.439685 7.465046 4.232334

27 H 8.086505 6.905049 5.459662 7.591558 4.225851

11 12 13 14 15

11 C 0.000000

12 C 1.531636 0.000000

13 C 2.546521 1.527236 0.000000

14 H 7.139968 8.329783 9.658834 0.000000

15 H 9.088027 10.532453 11.568501 3.949343 0.000000

16 H 5.714134 7.007175 8.166281 2.470431 4.793278

17 H 7.396206 8.738227 9.849755 2.525581 3.799262

18 H 6.259327 7.715070 8.709373 3.077787 3.543326

19 H 2.171592 2.818219 4.227684 5.911548 8.281507

20 H 2.169608 2.770117 4.204790 5.786772 8.546565

21 H 1.096749 2.157266 2.778509 7.256013 9.093756

22 H 1.095979 2.159795 2.766742 7.390220 8.910711

23 H 2.157597 1.096563 2.158271 8.428866 10.689248

24 H 2.157613 1.096393 2.158191 8.325656 10.847065

25 H 3.501007 2.180244 1.094285 10.502530 12.571121

26 H 2.813190 2.178658 1.095077 9.794812 11.619934

27 H 2.818088 2.179251 1.094982 9.887864 11.478428

16 17 18 19 20

16 H 0.000000

17 H 1.767525 0.000000

18 H 1.770088 1.772441 0.000000

19 H 5.211067 6.880404 5.943696 0.000000

20 H 4.594823 6.360405 5.680123 1.766835 0.000000

21 H 5.504778 7.140537 6.016996 3.073101 2.535287

22 H 6.071555 7.657407 6.329887 2.498057 3.070269

23 H 7.404084 9.133753 8.119303 2.584198 3.061612

24 H 6.956696 8.713402 7.881966 3.159601 2.547752

25 H 9.076319 10.789096 9.714955 4.918648 4.877728

26 H 8.071609 9.709620 8.585490 4.792408 4.448887

27 H 8.468106 10.096804 8.811911 4.434268 4.766073

21 22 23 24 25

21 H 0.000000

22 H 1.757424 0.000000

23 H 3.060711 2.516074 0.000000

24 H 2.499978 3.062214 1.754108 0.000000

25 H 3.781177 3.776419 2.504384 2.500476 0.000000

26 H 2.598095 3.121699 3.077665 2.526248 1.765617

27 H 3.150462 2.591235 2.523472 3.077819 1.765857

26 27

26 H 0.000000

27 H 1.765920 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.32D-01

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.118521 -0.425311 -0.161860

2 6 0 -2.848999 0.117694 0.429994

3 8 0 -4.897435 0.216845 -0.830251

4 8 0 -4.304133 -1.740074 0.089769

5 6 0 -2.354233 -0.573222 1.686440

6 16 0 -1.565159 0.022410 -0.972657

7 6 0 -0.115383 0.668314 -0.219104

8 16 0 1.096725 -0.591868 0.165812

9 16 0 -0.002035 2.293076 0.340788

10 6 0 2.691893 0.286477 -0.097697

11 6 0 3.859873 -0.689397 -0.008374

12 6 0 5.208699 0.018452 -0.168150

13 6 0 6.391627 -0.945493 -0.105367

14 1 0 -3.003403 1.182083 0.601664

15 1 0 -5.125232 -2.008126 -0.356316

16 1 0 -1.442189 -0.086931 2.035276

17 1 0 -3.101417 -0.499726 2.483278

18 1 0 -2.138911 -1.627867 1.512492

19 1 0 2.647213 0.756875 -1.082415

20 1 0 2.782166 1.074637 0.650363

21 1 0 3.837770 -1.209996 0.956689

22 1 0 3.758458 -1.460016 -0.781051

23 1 0 5.223331 0.556816 -1.123347

24 1 0 5.312501 0.779432 0.614291

25 1 0 7.344183 -0.418424 -0.216246

26 1 0 6.419731 -1.478915 0.850596

27 1 0 6.336099 -1.697001 -0.899809

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3281875 0.1918704 0.1799641

Leave Link 202 at Sat Aug 17 17:39:51 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1101.3609496420 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0549073307 Hartrees.

Nuclear repulsion after empirical dispersion term = 1101.3060423113 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2319

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.25D-08

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 103

GePol: Fraction of low-weight points (<1% of avg) = 4.44%

GePol: Cavity surface area = 309.457 Ang\*\*2

GePol: Cavity volume = 320.235 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057865454 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1101.3002557659 Hartrees.

Leave Link 301 at Sat Aug 17 17:39:51 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:39:51 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:39:52 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Lowest energy guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999999 0.001227 -0.000027 0.000067 Ang= 0.14 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999816 -0.019167 0.000318 -0.001171 Ang= -2.20 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 6.37D-02

Max alpha theta= 4.195 degrees.

Max beta theta= 4.206 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 17:39:52 2019, MaxMem= 1342177280 cpu: 4.2

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16133283.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.55D-15 for 2308.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.79D-15 for 584 302.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.33D-15 for 2309.

Iteration 1 A^-1\*A deviation from orthogonality is 2.37D-13 for 921 914.

E= -1658.67696390048

DIIS: error= 4.99D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67696390048 IErMin= 1 ErrMin= 4.99D-05

ErrMax= 4.99D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.07D-06 BMatP= 3.07D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 88.726 Goal= None Shift= 0.000

Gap= 88.741 Goal= None Shift= 0.000

RMSDP=4.52D-06 MaxDP=1.79D-04 OVMax= 2.73D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.51D-06 CP: 1.00D+00

E= -1658.67696425227 Delta-E= -0.000000351792 Rises=F Damp=F

DIIS: error= 5.82D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67696425227 IErMin= 1 ErrMin= 4.99D-05

ErrMax= 5.82D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.68D-06 BMatP= 3.07D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.478D+00 0.522D+00

Coeff: 0.478D+00 0.522D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.50D-06 MaxDP=1.65D-04 DE=-3.52D-07 OVMax= 2.11D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.22D-06 CP: 1.00D+00 7.50D-01

E= -1658.67696464292 Delta-E= -0.000000390656 Rises=F Damp=F

DIIS: error= 2.07D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67696464292 IErMin= 3 ErrMin= 2.07D-05

ErrMax= 2.07D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.13D-07 BMatP= 2.68D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.151D-01 0.319D+00 0.666D+00

Coeff: 0.151D-01 0.319D+00 0.666D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.05D-06 MaxDP=4.73D-05 DE=-3.91D-07 OVMax= 8.64D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 6.05D-07 CP: 1.00D+00 8.48D-01 6.69D-01

E= -1658.67696473857 Delta-E= -0.000000095648 Rises=F Damp=F

DIIS: error= 1.46D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67696473857 IErMin= 4 ErrMin= 1.46D-05

ErrMax= 1.46D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.66D-08 BMatP= 6.13D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.164D-01 0.179D+00 0.433D+00 0.404D+00

Coeff: -0.164D-01 0.179D+00 0.433D+00 0.404D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.82D-07 MaxDP=1.47D-05 DE=-9.56D-08 OVMax= 3.64D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.44D-07 CP: 1.00D+00 8.54D-01 7.34D-01 4.69D-01

E= -1658.67696475644 Delta-E= -0.000000017864 Rises=F Damp=F

DIIS: error= 2.00D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67696475644 IErMin= 5 ErrMin= 2.00D-06

ErrMax= 2.00D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.58D-09 BMatP= 9.66D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.927D-02 0.733D-01 0.182D+00 0.209D+00 0.544D+00

Coeff: -0.927D-02 0.733D-01 0.182D+00 0.209D+00 0.544D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.86D-08 MaxDP=4.15D-06 DE=-1.79D-08 OVMax= 5.65D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 6.35D-08 CP: 1.00D+00 8.56D-01 7.36D-01 4.79D-01 8.41D-01

E= -1658.67696475684 Delta-E= -0.000000000400 Rises=F Damp=F

DIIS: error= 3.38D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67696475684 IErMin= 6 ErrMin= 3.38D-07

ErrMax= 3.38D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.86D-10 BMatP= 2.58D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.149D-02 0.672D-02 0.186D-01 0.339D-01 0.237D+00 0.706D+00

Coeff: -0.149D-02 0.672D-02 0.186D-01 0.339D-01 0.237D+00 0.706D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.83D-08 MaxDP=1.13D-06 DE=-4.00D-10 OVMax= 2.83D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.93D-08 CP: 1.00D+00 8.57D-01 7.36D-01 4.96D-01 9.53D-01

CP: 9.00D-01

E= -1658.67696475691 Delta-E= -0.000000000071 Rises=F Damp=F

DIIS: error= 9.64D-08 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67696475691 IErMin= 7 ErrMin= 9.64D-08

ErrMax= 9.64D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.60D-11 BMatP= 1.86D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.448D-04-0.249D-02-0.506D-02 0.500D-04 0.745D-01 0.351D+00

Coeff-Com: 0.582D+00

Coeff: -0.448D-04-0.249D-02-0.506D-02 0.500D-04 0.745D-01 0.351D+00

Coeff: 0.582D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.57D-08 MaxDP=7.10D-07 DE=-7.09D-11 OVMax= 1.68D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.18D-08 CP: 1.00D+00 8.57D-01 7.39D-01 4.95D-01 9.82D-01

CP: 9.99D-01 8.62D-01

E= -1658.67696475688 Delta-E= 0.000000000028 Rises=F Damp=F

DIIS: error= 6.95D-08 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 7 EnMin= -1658.67696475691 IErMin= 8 ErrMin= 6.95D-08

ErrMax= 6.95D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.53D-12 BMatP= 2.60D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.353D-03-0.335D-02-0.805D-02-0.842D-02-0.839D-02 0.606D-01

Coeff-Com: 0.367D+00 0.600D+00

Coeff: 0.353D-03-0.335D-02-0.805D-02-0.842D-02-0.839D-02 0.606D-01

Coeff: 0.367D+00 0.600D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.92D-09 MaxDP=4.41D-07 DE= 2.77D-11 OVMax= 1.07D-06

Error on total polarization charges = 0.04170

SCF Done: E(UB3LYP) = -1658.67696476 A.U. after 8 cycles

NFock= 8 Conv=0.59D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655231926967D+03 PE=-6.145362424551D+03 EE= 1.730153277062D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.63

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:40:10 2019, MaxMem= 1342177280 cpu: 203.0

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 338

Leave Link 701 at Sat Aug 17 17:40:11 2019, MaxMem= 1342177280 cpu: 10.3

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:40:11 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:40:14 2019, MaxMem= 1342177280 cpu: 36.1

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.35264065D+00-2.90817229D+00 5.91162653D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000383255 -0.000340542 0.000425338

2 6 -0.000567808 -0.000468840 0.000077320

3 8 -0.000255963 0.000157128 -0.000232879

4 8 0.000186227 0.000194305 -0.000006406

5 6 0.000096082 -0.000106501 -0.000004555

6 16 0.000191743 0.000306172 -0.000082475

7 6 -0.000174982 0.000295718 -0.000021095

8 16 0.000465625 -0.000139864 0.000019188

9 16 -0.000167568 -0.000085492 0.000150540

10 6 -0.000218936 0.000037131 0.000021625

11 6 -0.000066690 -0.000171855 -0.000008052

12 6 -0.000068355 0.000134069 -0.000054646

13 6 0.000099948 -0.000146700 -0.000033007

14 1 0.000167424 0.000047710 -0.000136727

15 1 0.000008020 0.000202184 -0.000025733

16 1 0.000078667 -0.000011227 0.000042793

17 1 0.000050904 0.000023261 -0.000016606

18 1 -0.000035319 0.000057313 -0.000061345

19 1 0.000127652 0.000094994 0.000016670

20 1 -0.000169569 -0.000163783 0.000011060

21 1 -0.000033737 0.000069108 -0.000036047

22 1 0.000029150 0.000003091 -0.000014591

23 1 -0.000002939 -0.000026572 0.000051286

24 1 0.000033510 -0.000062992 0.000015134

25 1 -0.000075983 0.000015442 -0.000027172

26 1 -0.000017006 0.000020530 -0.000071768

27 1 -0.000063354 0.000066213 0.000002151

-------------------------------------------------------------------

Cartesian Forces: Max 0.000567808 RMS 0.000162991

Leave Link 716 at Sat Aug 17 17:40:14 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000930831 RMS 0.000178090

Search for a local minimum.

Step number 23 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .17809D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

19

ITU= 0 -1 1 -1 1 -1 1 1 -1 1 -1 1 1 -1 0 0 -1 0 0 -1

ITU= -1 0 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.88246.

Iteration 1 RMS(Cart)= 0.00575704 RMS(Int)= 0.00001650

Iteration 2 RMS(Cart)= 0.00003095 RMS(Int)= 0.00000003

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000003

ITry= 1 IFail=0 DXMaxC= 2.89D-02 DCOld= 1.00D+10 DXMaxT= 5.95D-02 DXLimC= 3.00D+00 Rises=T

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83889 -0.00040 -0.00111 0.00000 -0.00111 2.83779

R2 2.28791 0.00036 0.00026 0.00000 0.00026 2.28817

R3 2.55384 -0.00037 -0.00051 0.00000 -0.00051 2.55333

R4 2.86642 -0.00001 0.00021 0.00000 0.00021 2.86663

R5 3.59781 -0.00001 -0.00079 0.00000 -0.00079 3.59702

R6 2.05818 -0.00002 -0.00005 0.00000 -0.00005 2.05814

R7 1.83707 -0.00005 -0.00003 0.00000 -0.00003 1.83704

R8 2.06144 0.00009 0.00003 0.00000 0.00003 2.06147

R9 2.06891 -0.00004 -0.00009 0.00000 -0.00009 2.06882

R10 2.06049 -0.00008 -0.00011 0.00000 -0.00011 2.06038

R11 3.32016 -0.00027 0.00019 0.00000 0.00019 3.32035

R12 3.38331 0.00026 0.00054 0.00000 0.00054 3.38385

R13 3.25460 -0.00004 -0.00037 0.00000 -0.00037 3.25423

R14 3.47704 -0.00045 -0.00050 0.00000 -0.00050 3.47654

R15 2.88113 -0.00003 -0.00009 0.00000 -0.00009 2.88104

R16 2.06399 0.00004 -0.00016 0.00000 -0.00016 2.06383

R17 2.06053 -0.00012 -0.00016 0.00000 -0.00016 2.06036

R18 2.89437 -0.00009 -0.00004 0.00000 -0.00004 2.89434

R19 2.07255 -0.00005 -0.00013 0.00000 -0.00013 2.07243

R20 2.07110 0.00000 -0.00013 0.00000 -0.00013 2.07097

R21 2.88606 0.00000 -0.00010 0.00000 -0.00010 2.88596

R22 2.07220 -0.00006 -0.00012 0.00000 -0.00012 2.07208

R23 2.07188 -0.00003 -0.00009 0.00000 -0.00009 2.07179

R24 2.06790 -0.00006 -0.00014 0.00000 -0.00014 2.06776

R25 2.06940 -0.00005 -0.00012 0.00000 -0.00012 2.06928

R26 2.06922 -0.00006 -0.00012 0.00000 -0.00012 2.06910

A1 2.17664 0.00020 0.00046 0.00000 0.00046 2.17710

A2 1.97616 -0.00015 -0.00008 0.00000 -0.00008 1.97608

A3 2.12991 -0.00005 -0.00043 0.00000 -0.00043 2.12948

A4 2.02344 0.00002 -0.00009 0.00000 -0.00009 2.02335

A5 1.83538 0.00015 0.00193 0.00000 0.00193 1.83731

A6 1.87081 0.00007 0.00046 0.00000 0.00046 1.87127

A7 1.94712 -0.00012 -0.00055 0.00000 -0.00055 1.94658

A8 1.93995 0.00002 0.00007 0.00000 0.00007 1.94002

A9 1.83447 -0.00013 -0.00191 0.00000 -0.00191 1.83256

A10 1.87425 -0.00030 -0.00078 0.00000 -0.00078 1.87347

A11 1.91191 0.00001 -0.00032 0.00000 -0.00032 1.91159

A12 1.92804 -0.00002 0.00047 0.00000 0.00047 1.92850

A13 1.95287 -0.00006 -0.00045 0.00000 -0.00045 1.95242

A14 1.88381 -0.00001 -0.00002 0.00000 -0.00002 1.88379

A15 1.89346 0.00003 -0.00013 0.00000 -0.00013 1.89332

A16 1.89211 0.00006 0.00047 0.00000 0.00047 1.89258

A17 1.79471 -0.00093 -0.00145 0.00000 -0.00145 1.79326

A18 1.97371 -0.00056 -0.00121 0.00000 -0.00121 1.97249

A19 2.14189 0.00006 0.00003 0.00000 0.00003 2.14192

A20 2.15265 0.00040 0.00110 0.00000 0.00110 2.15375

A21 1.79276 0.00056 0.00006 0.00000 0.00006 1.79282

A22 1.92859 -0.00054 0.00010 0.00000 0.00010 1.92869

A23 1.87470 0.00028 -0.00019 0.00000 -0.00019 1.87451

A24 1.89503 0.00005 0.00019 0.00000 0.00019 1.89522

A25 1.93888 0.00006 -0.00030 0.00000 -0.00030 1.93858

A26 1.93804 0.00020 0.00029 0.00000 0.00029 1.93833

A27 1.88663 -0.00004 -0.00011 0.00000 -0.00011 1.88652

A28 1.95273 0.00014 -0.00033 0.00000 -0.00033 1.95240

A29 1.91765 -0.00010 0.00037 0.00000 0.00037 1.91802

A30 1.91544 0.00000 -0.00019 0.00000 -0.00019 1.91525

A31 1.90595 0.00001 0.00003 0.00000 0.00003 1.90597

A32 1.91017 -0.00010 0.00003 0.00000 0.00003 1.91020

A33 1.85953 0.00003 0.00012 0.00000 0.00012 1.85965

A34 1.96722 -0.00016 0.00009 0.00000 0.00009 1.96731

A35 1.90659 0.00003 -0.00019 0.00000 -0.00019 1.90639

A36 1.90678 0.00008 0.00003 0.00000 0.00003 1.90681

A37 1.91277 0.00004 -0.00002 0.00000 -0.00002 1.91275

A38 1.91284 0.00002 -0.00006 0.00000 -0.00006 1.91278

A39 1.85420 -0.00001 0.00015 0.00000 0.00015 1.85435

A40 1.94557 -0.00005 -0.00029 0.00000 -0.00029 1.94528

A41 1.94251 -0.00001 -0.00017 0.00000 -0.00017 1.94234

A42 1.94344 -0.00006 0.00016 0.00000 0.00016 1.94360

A43 1.87626 0.00004 0.00017 0.00000 0.00017 1.87643

A44 1.87675 0.00006 0.00024 0.00000 0.00024 1.87699

A45 1.87586 0.00003 -0.00010 0.00000 -0.00010 1.87576

D1 2.67340 0.00007 -0.00542 0.00000 -0.00542 2.66798

D2 -1.45043 0.00004 -0.00471 0.00000 -0.00471 -1.45514

D3 0.49558 -0.00001 -0.00582 0.00000 -0.00582 0.48975

D4 -0.50053 0.00003 -0.00735 0.00000 -0.00735 -0.50788

D5 1.65882 -0.00001 -0.00663 0.00000 -0.00663 1.65219

D6 -2.67836 -0.00006 -0.00774 0.00000 -0.00774 -2.68610

D7 -3.10486 0.00000 0.00088 0.00000 0.00088 -3.10399

D8 0.00537 -0.00004 -0.00097 0.00000 -0.00097 0.00440

D9 -3.12366 -0.00001 0.00373 0.00000 0.00373 -3.11993

D10 -1.05076 -0.00004 0.00379 0.00000 0.00379 -1.04697

D11 1.05903 -0.00002 0.00441 0.00000 0.00441 1.06344

D12 1.05952 -0.00012 0.00166 0.00000 0.00166 1.06117

D13 3.13243 -0.00015 0.00171 0.00000 0.00171 3.13414

D14 -1.04097 -0.00013 0.00233 0.00000 0.00233 -1.03864

D15 -0.98182 0.00011 0.00434 0.00000 0.00434 -0.97748

D16 1.09109 0.00009 0.00440 0.00000 0.00440 1.09549

D17 -3.08231 0.00011 0.00501 0.00000 0.00501 -3.07729

D18 3.14117 0.00028 -0.00884 0.00000 -0.00884 3.13233

D19 -0.93487 0.00033 -0.00796 0.00000 -0.00796 -0.94282

D20 1.16942 0.00020 -0.00935 0.00000 -0.00935 1.16007

D21 1.84896 -0.00035 -0.00120 0.00000 -0.00120 1.84777

D22 -1.11325 0.00018 -0.00081 0.00000 -0.00081 -1.11406

D23 2.54657 0.00028 0.00084 0.00000 0.00084 2.54741

D24 -0.77568 -0.00030 0.00033 0.00000 0.00033 -0.77535

D25 -3.00095 -0.00005 0.01074 0.00000 0.01074 -2.99021

D26 -0.88347 -0.00011 0.01032 0.00000 0.01032 -0.87315

D27 1.15277 0.00001 0.01019 0.00000 0.01019 1.16297

D28 -3.10219 0.00001 -0.00033 0.00000 -0.00033 -3.10252

D29 -0.98210 0.00005 -0.00027 0.00000 -0.00027 -0.98237

D30 1.05707 0.00004 -0.00002 0.00000 -0.00002 1.05706

D31 1.10199 -0.00003 0.00003 0.00000 0.00003 1.10203

D32 -3.06110 0.00001 0.00010 0.00000 0.00010 -3.06100

D33 -1.02193 0.00000 0.00035 0.00000 0.00035 -1.02158

D34 -0.99824 -0.00015 0.00017 0.00000 0.00017 -0.99807

D35 1.12185 -0.00011 0.00024 0.00000 0.00024 1.12208

D36 -3.12216 -0.00013 0.00049 0.00000 0.00049 -3.12167

D37 -3.12461 -0.00001 -0.00122 0.00000 -0.00122 -3.12583

D38 -0.99387 -0.00004 -0.00132 0.00000 -0.00132 -0.99520

D39 1.02761 0.00001 -0.00123 0.00000 -0.00123 1.02638

D40 1.03175 0.00001 -0.00149 0.00000 -0.00149 1.03026

D41 -3.12070 -0.00002 -0.00159 0.00000 -0.00159 -3.12228

D42 -1.09921 0.00003 -0.00150 0.00000 -0.00150 -1.10071

D43 -0.99766 0.00002 -0.00167 0.00000 -0.00167 -0.99933

D44 1.13307 -0.00001 -0.00176 0.00000 -0.00176 1.13131

D45 -3.12862 0.00004 -0.00168 0.00000 -0.00168 -3.13030

D46 -3.13630 -0.00003 -0.00209 0.00000 -0.00209 -3.13840

D47 -1.04168 -0.00002 -0.00218 0.00000 -0.00218 -1.04386

D48 1.05100 -0.00003 -0.00231 0.00000 -0.00231 1.04869

D49 1.01963 0.00001 -0.00189 0.00000 -0.00189 1.01774

D50 3.11426 0.00002 -0.00199 0.00000 -0.00199 3.11227

D51 -1.07625 0.00001 -0.00212 0.00000 -0.00212 -1.07836

D52 -1.00876 -0.00002 -0.00203 0.00000 -0.00203 -1.01079

D53 1.08586 -0.00001 -0.00212 0.00000 -0.00212 1.08374

D54 -3.10465 -0.00002 -0.00225 0.00000 -0.00225 -3.10690

Item Value Threshold Converged?

Maximum Force 0.000931 0.000450 NO

RMS Force 0.000178 0.000300 YES

Maximum Displacement 0.028871 0.001800 NO

RMS Displacement 0.005761 0.001200 NO

Predicted change in Energy=-1.563792D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:40:14 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.105742 -0.410019 -0.214789

2 6 0 -2.840357 0.052498 0.448502

3 8 0 -4.883754 0.312699 -0.796625

4 8 0 -4.288140 -1.746769 -0.140816

5 6 0 -2.353228 -0.792628 1.610236

6 16 0 -1.546130 0.137276 -0.944680

7 6 0 -0.107821 0.695923 -0.104191

8 16 0 1.108868 -0.595777 0.135870

9 16 0 -0.011508 2.240995 0.650123

10 6 0 2.700600 0.316298 -0.002045

11 6 0 3.872997 -0.657689 -0.036333

12 6 0 5.218667 0.071364 -0.095534

13 6 0 6.406542 -0.886741 -0.152797

14 1 0 -2.995262 1.086759 0.752618

15 1 0 -5.106556 -1.954640 -0.622480

16 1 0 -1.445460 -0.352827 2.025640

17 1 0 -3.106523 -0.823670 2.404033

18 1 0 -2.132764 -1.815525 1.303887

19 1 0 2.657755 0.911576 -0.916681

20 1 0 2.783805 0.999925 0.843225

21 1 0 3.849933 -1.300861 0.851648

22 1 0 3.778471 -1.320192 -0.904192

23 1 0 5.234527 0.729522 -0.972396

24 1 0 5.314853 0.724347 0.779873

25 1 0 7.356362 -0.344835 -0.191239

26 1 0 6.434388 -1.538458 0.726719

27 1 0 6.357637 -1.530187 -1.037350

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.501692 0.000000

3 O 1.210849 2.406973 0.000000

4 O 1.351163 2.383429 2.241930 0.000000

5 C 2.558986 1.516956 3.663098 2.778570 0.000000

6 S 2.717330 1.903462 3.345508 3.422636 2.836146

7 C 4.149543 2.861156 4.841059 4.841812 3.193258

8 S 5.229687 4.014271 6.132405 5.525308 3.768105

9 S 4.953655 3.582256 5.436008 5.900629 3.950739

10 C 6.848291 5.565499 7.625863 7.288208 5.419441

11 C 7.984577 6.768202 8.843098 8.234146 6.441683

12 C 9.337588 8.077387 10.129594 9.679206 7.809592

13 C 10.523270 9.313907 11.372069 10.729213 8.935923

14 H 2.099854 1.089118 2.562367 3.240161 2.163287

15 H 1.885125 3.211116 2.284906 0.972119 3.730430

16 H 3.478490 2.144152 4.497774 3.836331 1.090884

17 H 2.833333 2.159309 3.833288 2.953741 1.094774

18 H 2.859102 2.172989 4.063180 2.595677 1.090308

19 H 6.927060 5.729831 7.566203 7.477581 5.865115

20 H 7.111483 5.717046 7.871013 7.650167 5.494603

21 H 8.076116 6.837695 9.033142 8.210483 6.270005

22 H 7.966461 6.893688 8.815444 8.113872 6.648188

23 H 9.439976 8.226849 10.128388 9.874448 8.158489

24 H 9.540637 8.189544 10.327942 9.958492 7.860674

25 H 11.462313 10.224491 12.272704 11.728699 9.885442

26 H 10.642093 9.414320 11.569256 10.759582 8.863355

27 H 10.555268 9.450700 11.393991 10.685656 9.134160

6 7 8 9 10

6 S 0.000000

7 C 1.757055 0.000000

8 S 2.958711 1.790657 0.000000

9 S 3.053539 1.722067 3.093053 0.000000

10 C 4.353772 2.835803 1.839704 3.388998 0.000000

11 C 5.551938 4.205210 2.770180 4.895199 1.524580

12 C 6.818202 5.362986 4.170020 5.711219 2.531678

13 C 8.057337 6.704037 5.313505 7.184621 3.899235

14 H 2.425350 3.037135 4.478302 3.200868 5.797065

15 H 4.142047 5.681677 6.407269 6.721784 8.154372

16 H 3.012165 2.724946 3.186667 3.267442 4.663587

17 H 3.817345 4.194349 4.792287 4.695476 6.388381

18 H 3.035395 3.520006 3.655164 4.624120 5.441648

19 H 4.274690 2.890512 2.403960 3.368559 1.092131

20 H 4.763308 3.058025 2.419097 3.064525 1.090298

21 H 5.866219 4.534820 2.919403 5.243671 2.159852

22 H 5.520619 4.450616 2.955213 5.427880 2.157261

23 H 6.806529 5.412540 4.472777 5.695436 2.744653

24 H 7.098721 5.494341 4.455085 5.539601 2.759025

25 H 8.947316 7.536895 6.261082 7.853656 4.706273

26 H 8.324081 6.963000 5.440488 7.472597 4.232303

27 H 8.078277 6.901340 5.458859 7.591797 4.225551

11 12 13 14 15

11 C 0.000000

12 C 1.531616 0.000000

13 C 2.546542 1.527185 0.000000

14 H 7.130114 8.319796 9.649269 0.000000

15 H 9.091646 10.535302 11.572054 3.949502 0.000000

16 H 5.712325 7.006418 8.166063 2.468781 4.793951

17 H 7.395717 8.738289 9.850876 2.527705 3.799869

18 H 6.261465 7.717659 8.712308 3.077507 3.545938

19 H 2.171271 2.817536 4.227395 5.896935 8.281682

20 H 2.169711 2.769846 4.204259 5.780429 8.551931

21 H 1.096682 2.157218 2.777887 7.250326 9.100503

22 H 1.095912 2.159750 2.767531 7.377119 8.912103

23 H 2.157390 1.096499 2.158164 8.416217 10.689488

24 H 2.157583 1.096346 2.158069 8.318059 10.851237

25 H 3.500814 2.179936 1.094211 10.492685 12.573852

26 H 2.814022 2.178441 1.095015 9.788295 11.626991

27 H 2.817219 2.179275 1.094919 9.875683 11.479546

16 17 18 19 20

16 H 0.000000

17 H 1.767485 0.000000

18 H 1.769971 1.772654 0.000000

19 H 5.205030 6.874963 5.942817 0.000000

20 H 4.595076 6.360627 5.684331 1.766625 0.000000

21 H 5.506197 7.143520 6.021799 3.072971 2.535807

22 H 6.067055 7.654673 6.329587 2.497388 3.070141

23 H 7.401481 9.131582 8.120080 2.583796 3.061966

24 H 6.958022 8.715149 7.886225 3.158089 2.546795

25 H 9.076711 10.790582 9.718119 4.917493 4.877169

26 H 8.073717 9.713561 8.591041 4.792326 4.447889

27 H 8.465010 10.095177 8.811908 4.434624 4.765533

21 22 23 24 25

21 H 0.000000

22 H 1.757399 0.000000

23 H 3.060505 2.515169 0.000000

24 H 2.500523 3.062137 1.754117 0.000000

25 H 3.781090 3.776364 2.503325 2.500793 0.000000

26 H 2.598359 3.124324 3.077400 2.525167 1.765621

27 H 3.147933 2.591124 2.524258 3.077762 1.765903

26 27

26 H 0.000000

27 H 1.765758 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 7.84D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.118639 -0.421540 -0.162309

2 6 0 -2.846222 0.112880 0.429660

3 8 0 -4.897717 0.227551 -0.824030

4 8 0 -4.306534 -1.737749 0.078383

5 6 0 -2.354215 -0.584083 1.683984

6 16 0 -1.562129 0.016975 -0.972151

7 6 0 -0.115028 0.667844 -0.217492

8 16 0 1.097562 -0.590639 0.172758

9 16 0 -0.006046 2.294077 0.338387

10 6 0 2.692332 0.288593 -0.088344

11 6 0 3.860011 -0.688467 -0.009468

12 6 0 5.208489 0.020273 -0.168039

13 6 0 6.391544 -0.943966 -0.114040

14 1 0 -2.994148 1.177725 0.604017

15 1 0 -5.129480 -1.999372 -0.368080

16 1 0 -1.441367 -0.101042 2.035278

17 1 0 -3.101657 -0.512225 2.480663

18 1 0 -2.140699 -1.638286 1.505548

19 1 0 2.645315 0.765914 -1.069518

20 1 0 2.784983 1.071426 0.664874

21 1 0 3.840703 -1.216264 0.951661

22 1 0 3.755964 -1.453084 -0.787645

23 1 0 5.220743 0.564359 -1.119948

24 1 0 5.314209 0.776371 0.618799

25 1 0 7.343495 -0.416195 -0.226039

26 1 0 6.423043 -1.481568 0.839402

27 1 0 6.333078 -1.691994 -0.911463

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3290284 0.1918992 0.1799617

Leave Link 202 at Sat Aug 17 17:40:14 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1101.4211817162 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0549134722 Hartrees.

Nuclear repulsion after empirical dispersion term = 1101.3662682440 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2318

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.89D-08

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 103

GePol: Fraction of low-weight points (<1% of avg) = 4.44%

GePol: Cavity surface area = 309.455 Ang\*\*2

GePol: Cavity volume = 320.176 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0058008294 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1101.3604674146 Hartrees.

Leave Link 301 at Sat Aug 17 17:40:14 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:40:14 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:40:14 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Lowest energy guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000144 -0.000003 0.000008 Ang= 0.02 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999999 -0.001083 0.000024 -0.000059 Ang= -0.12 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 1.18D-01

Max alpha theta= 0.265 degrees.

Max beta theta= 0.266 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 17:40:15 2019, MaxMem= 1342177280 cpu: 4.3

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16119372.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.33D-15 for 2308.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.52D-15 for 706 445.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.33D-15 for 2308.

Iteration 1 A^-1\*A deviation from orthogonality is 1.24D-12 for 918 911.

E= -1658.67697344522

DIIS: error= 3.68D-07 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67697344522 IErMin= 1 ErrMin= 3.68D-07

ErrMax= 3.68D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.62D-10 BMatP= 1.62D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 88.739 Goal= None Shift= 0.000

Gap= 88.754 Goal= None Shift= 0.000

RMSDP=3.31D-08 MaxDP=1.39D-06 OVMax= 2.12D-06

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.30D-08 CP: 1.00D+00

E= -1658.67697344525 Delta-E= -0.000000000032 Rises=F Damp=F

DIIS: error= 4.37D-07 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67697344525 IErMin= 1 ErrMin= 3.68D-07

ErrMax= 4.37D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.47D-10 BMatP= 1.62D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.484D+00 0.516D+00

Coeff: 0.484D+00 0.516D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.80D-08 MaxDP=1.21D-06 DE=-3.18D-11 OVMax= 1.55D-06

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.58D-08 CP: 1.00D+00 7.39D-01

E= -1658.67697344523 Delta-E= 0.000000000018 Rises=F Damp=F

DIIS: error= 1.44D-07 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1658.67697344525 IErMin= 3 ErrMin= 1.44D-07

ErrMax= 1.44D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.97D-11 BMatP= 1.47D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.169D-01 0.306D+00 0.678D+00

Coeff: 0.169D-01 0.306D+00 0.678D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=7.42D-09 MaxDP=3.42D-07 DE= 1.82D-11 OVMax= 6.44D-07

Error on total polarization charges = 0.04170

SCF Done: E(UB3LYP) = -1658.67697345 A.U. after 3 cycles

NFock= 3 Conv=0.74D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655235108593D+03 PE=-6.145484098099D+03 EE= 1.730211548647D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.64

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:40:24 2019, MaxMem= 1342177280 cpu: 96.3

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 338

Leave Link 701 at Sat Aug 17 17:40:25 2019, MaxMem= 1342177280 cpu: 10.2

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:40:25 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:40:28 2019, MaxMem= 1342177280 cpu: 36.1

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.35751886D+00-2.91053909D+00 5.87893820D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000282505 -0.000168265 -0.000021244

2 6 -0.000378915 -0.000272173 0.000295043

3 8 -0.000200518 0.000146053 -0.000084662

4 8 0.000099129 0.000006032 0.000051702

5 6 0.000133910 -0.000021767 -0.000037296

6 16 0.000141232 0.000288409 -0.000125294

7 6 -0.000138635 0.000120185 -0.000127451

8 16 0.000381384 -0.000050551 -0.000001369

9 16 -0.000076673 -0.000094745 0.000216217

10 6 -0.000217176 0.000010780 -0.000019553

11 6 -0.000036502 -0.000093274 0.000018632

12 6 -0.000067728 0.000075956 -0.000071955

13 6 0.000045321 -0.000109548 0.000005068

14 1 0.000073530 0.000032658 -0.000078405

15 1 -0.000010259 0.000103137 -0.000001193

16 1 0.000071655 -0.000040695 0.000056558

17 1 0.000017771 0.000012494 -0.000007218

18 1 -0.000057094 -0.000003281 -0.000034544

19 1 0.000109220 0.000116383 -0.000014267

20 1 -0.000127158 -0.000109422 0.000053270

21 1 -0.000047146 0.000048933 0.000009793

22 1 0.000032887 -0.000024397 -0.000026349

23 1 0.000000488 0.000003533 0.000020758

24 1 0.000034371 -0.000034110 0.000025429

25 1 -0.000019645 0.000008550 -0.000026077

26 1 0.000001916 -0.000002259 -0.000037729

27 1 -0.000047870 0.000051383 -0.000037864

-------------------------------------------------------------------

Cartesian Forces: Max 0.000381384 RMS 0.000116257

Leave Link 716 at Sat Aug 17 17:40:28 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000665118 RMS 0.000136863

Search for a local minimum.

Step number 24 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .13686D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 19

23 24

ITU= 0 0 -1 1 -1 1 -1 1 1 -1 1 -1 1 1 -1 0 0 -1 0 0

ITU= -1 -1 0 0

Eigenvalues --- 0.00000 0.00001 0.00134 0.00260 0.00351

Eigenvalues --- 0.00426 0.00540 0.00968 0.01083 0.01679

Eigenvalues --- 0.02341 0.03475 0.03597 0.04274 0.04661

Eigenvalues --- 0.04739 0.04821 0.04985 0.05118 0.05460

Eigenvalues --- 0.05482 0.05526 0.05714 0.05892 0.08129

Eigenvalues --- 0.08239 0.08365 0.11299 0.11828 0.12240

Eigenvalues --- 0.13945 0.15167 0.15402 0.15982 0.16005

Eigenvalues --- 0.16057 0.16085 0.16564 0.16779 0.17303

Eigenvalues --- 0.18638 0.21543 0.21916 0.22145 0.22427

Eigenvalues --- 0.24240 0.24578 0.24939 0.25664 0.26183

Eigenvalues --- 0.26911 0.27774 0.29085 0.29468 0.29736

Eigenvalues --- 0.30162 0.30975 0.32310 0.33451 0.33873

Eigenvalues --- 0.33882 0.33925 0.33959 0.34019 0.34038

Eigenvalues --- 0.34110 0.34164 0.34351 0.34491 0.34575

Eigenvalues --- 0.34646 0.38639 0.52782 0.55321 1.12537

Eigenvalue 1 is 3.14D-07 Eigenvector:

D25 D26 D27 D6 D4

1 -0.33215 -0.32547 -0.31818 -0.25711 -0.24842

D5 D18 D19 D20 D3

1 -0.24544 0.24520 0.24506 0.22832 -0.19619

Eigenvalue 2 is 1.15D-05 Eigenvector:

D19 D20 D18 D1 D3

1 0.33602 0.33576 0.33381 0.33369 0.31354

D2 D4 D6 D5 D24

1 0.31223 0.22443 0.20428 0.20297 0.14759

En-DIIS/RFO-DIIS IScMMF= 0 using points: 24 23

RFO step: Lambda=-3.21713370D-05.

NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=F DC= 8.69D-06 SmlDif= 1.00D-05

RMS Error= 0.4496749007D-02 NUsed= 2 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.27322 0.72678

Iteration 1 RMS(Cart)= 0.45293291 RMS(Int)= 0.38089598

Iteration 2 RMS(Cart)= 0.47332162 RMS(Int)= 0.31074498

Iteration 3 RMS(Cart)= 0.39232338 RMS(Int)= 0.24894278

Iteration 4 RMS(Cart)= 0.34100749 RMS(Int)= 0.19961497

Iteration 5 RMS(Cart)= 0.26397290 RMS(Int)= 0.15377738

Iteration 6 RMS(Cart)= 0.22007111 RMS(Int)= 0.10936934

Iteration 7 RMS(Cart)= 0.21251375 RMS(Int)= 0.06643157

Iteration 8 RMS(Cart)= 0.20767394 RMS(Int)= 0.02751623

Iteration 9 RMS(Cart)= 0.14574787 RMS(Int)= 0.00804362

Iteration 10 RMS(Cart)= 0.00964173 RMS(Int)= 0.00597561

Iteration 11 RMS(Cart)= 0.00001608 RMS(Int)= 0.00597559

Iteration 12 RMS(Cart)= 0.00000034 RMS(Int)= 0.00597559

ITry= 1 IFail=0 DXMaxC= 9.43D+00 DCOld= 1.00D+10 DXMaxT= 5.95D-02 DXLimC= 3.00D+00 Rises=F

Iteration 1 RMS(Cart)= 0.43888972 RMS(Int)= 0.33605051

Iteration 2 RMS(Cart)= 0.46086455 RMS(Int)= 0.26753873

Iteration 3 RMS(Cart)= 0.37048311 RMS(Int)= 0.20909092

Iteration 4 RMS(Cart)= 0.32295791 RMS(Int)= 0.16155557

Iteration 5 RMS(Cart)= 0.23371971 RMS(Int)= 0.11634013

Iteration 6 RMS(Cart)= 0.21336396 RMS(Int)= 0.07278482

Iteration 7 RMS(Cart)= 0.20802852 RMS(Int)= 0.03186013

Iteration 8 RMS(Cart)= 0.16537430 RMS(Int)= 0.00845563

Iteration 9 RMS(Cart)= 0.01256541 RMS(Int)= 0.00481497

Iteration 10 RMS(Cart)= 0.00003167 RMS(Int)= 0.00481490

Iteration 11 RMS(Cart)= 0.00000035 RMS(Int)= 0.00481490

ITry= 2 IFail=0 DXMaxC= 8.61D+00 DCOld= 9.43D+00 DXMaxT= 5.95D-02 DXLimC= 3.00D+00 Rises=F

Iteration 1 RMS(Cart)= 0.42303135 RMS(Int)= 0.29168015

Iteration 2 RMS(Cart)= 0.43971780 RMS(Int)= 0.22433828

Iteration 3 RMS(Cart)= 0.34926390 RMS(Int)= 0.16966348

Iteration 4 RMS(Cart)= 0.27714640 RMS(Int)= 0.12347767

Iteration 5 RMS(Cart)= 0.22081289 RMS(Int)= 0.07923684

Iteration 6 RMS(Cart)= 0.20873096 RMS(Int)= 0.03694572

Iteration 7 RMS(Cart)= 0.18239280 RMS(Int)= 0.00905498

Iteration 8 RMS(Cart)= 0.01587688 RMS(Int)= 0.00378387

Iteration 9 RMS(Cart)= 0.00009791 RMS(Int)= 0.00378366

Iteration 10 RMS(Cart)= 0.00000028 RMS(Int)= 0.00378366

ITry= 3 IFail=0 DXMaxC= 7.67D+00 DCOld= 8.61D+00 DXMaxT= 5.95D-02 DXLimC= 3.00D+00 Rises=F

Iteration 1 RMS(Cart)= 0.40722758 RMS(Int)= 0.24792310

Iteration 2 RMS(Cart)= 0.41126276 RMS(Int)= 0.18264341

Iteration 3 RMS(Cart)= 0.33461076 RMS(Int)= 0.13162584

Iteration 4 RMS(Cart)= 0.24041231 RMS(Int)= 0.08635372

Iteration 5 RMS(Cart)= 0.20966079 RMS(Int)= 0.04318965

Iteration 6 RMS(Cart)= 0.18834064 RMS(Int)= 0.00991158

Iteration 7 RMS(Cart)= 0.03331948 RMS(Int)= 0.00289340

Iteration 8 RMS(Cart)= 0.00057651 RMS(Int)= 0.00288034

Iteration 9 RMS(Cart)= 0.00000015 RMS(Int)= 0.00288034

ITry= 4 IFail=0 DXMaxC= 6.62D+00 DCOld= 7.67D+00 DXMaxT= 5.95D-02 DXLimC= 3.00D+00 Rises=F

Iteration 1 RMS(Cart)= 0.39188958 RMS(Int)= 0.20453624

Iteration 2 RMS(Cart)= 0.38106413 RMS(Int)= 0.14282254

Iteration 3 RMS(Cart)= 0.29155936 RMS(Int)= 0.09426136

Iteration 4 RMS(Cart)= 0.21973898 RMS(Int)= 0.05029396

Iteration 5 RMS(Cart)= 0.19636278 RMS(Int)= 0.01262075

Iteration 6 RMS(Cart)= 0.05774000 RMS(Int)= 0.00228729

Iteration 7 RMS(Cart)= 0.00162549 RMS(Int)= 0.00210331

Iteration 8 RMS(Cart)= 0.00000074 RMS(Int)= 0.00210331

ITry= 5 IFail=0 DXMaxC= 5.50D+00 DCOld= 6.62D+00 DXMaxT= 5.95D-02 DXLimC= 3.00D+00 Rises=F

Iteration 1 RMS(Cart)= 0.37386366 RMS(Int)= 0.16166260

Iteration 2 RMS(Cart)= 0.34323539 RMS(Int)= 0.10406216

Iteration 3 RMS(Cart)= 0.25017165 RMS(Int)= 0.05776748

Iteration 4 RMS(Cart)= 0.20328570 RMS(Int)= 0.01659916

Iteration 5 RMS(Cart)= 0.07923570 RMS(Int)= 0.00218910

Iteration 6 RMS(Cart)= 0.00300452 RMS(Int)= 0.00145093

Iteration 7 RMS(Cart)= 0.00000280 RMS(Int)= 0.00145093

Iteration 8 RMS(Cart)= 0.00000000 RMS(Int)= 0.00145093

ITry= 6 IFail=0 DXMaxC= 4.36D+00 DCOld= 5.50D+00 DXMaxT= 5.95D-02 DXLimC= 3.00D+00 Rises=F

Iteration 1 RMS(Cart)= 0.34728734 RMS(Int)= 0.11842401

Iteration 2 RMS(Cart)= 0.30971699 RMS(Int)= 0.06620420

Iteration 3 RMS(Cart)= 0.21672546 RMS(Int)= 0.02198539

Iteration 4 RMS(Cart)= 0.09822171 RMS(Int)= 0.00248962

Iteration 5 RMS(Cart)= 0.00463048 RMS(Int)= 0.00092151

Iteration 6 RMS(Cart)= 0.00000898 RMS(Int)= 0.00092150

Iteration 7 RMS(Cart)= 0.00000000 RMS(Int)= 0.00092150

ITry= 7 IFail=0 DXMaxC= 3.24D+00 DCOld= 4.36D+00 DXMaxT= 5.95D-02 DXLimC= 3.00D+00 Rises=F

Iteration 1 RMS(Cart)= 0.31624553 RMS(Int)= 0.07759316

Iteration 2 RMS(Cart)= 0.25424728 RMS(Int)= 0.02946349

Iteration 3 RMS(Cart)= 0.13110754 RMS(Int)= 0.00392842

Iteration 4 RMS(Cart)= 0.00846868 RMS(Int)= 0.00051353

Iteration 5 RMS(Cart)= 0.00003491 RMS(Int)= 0.00051336

Iteration 6 RMS(Cart)= 0.00000000 RMS(Int)= 0.00051336

ITry= 8 IFail=0 DXMaxC= 2.20D+00 DCOld= 3.24D+00 DXMaxT= 5.95D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83779 -0.00014 0.00080 -0.12099 -0.03549 2.80229

R2 2.28817 0.00025 -0.00019 -0.14817 -0.04464 2.24353

R3 2.55333 -0.00007 0.00037 -0.08389 -0.02480 2.52853

R4 2.86663 0.00001 -0.00015 -0.02144 -0.00659 2.86005

R5 3.59702 0.00010 0.00057 -0.01610 -0.00426 3.59276

R6 2.05814 0.00000 0.00004 -0.05937 -0.01778 2.04036

R7 1.83704 -0.00003 0.00002 -0.06559 -0.01966 1.81738

R8 2.06147 0.00008 -0.00002 -0.04069 -0.01223 2.04924

R9 2.06882 -0.00001 0.00007 -0.04552 -0.01359 2.05523

R10 2.06038 -0.00003 0.00008 -0.04507 -0.01344 2.04694

R11 3.32035 -0.00019 -0.00014 -0.03190 -0.00971 3.31064

R12 3.38385 0.00015 -0.00039 0.07047 0.02075 3.40460

R13 3.25423 -0.00002 0.00027 -0.06740 -0.01996 3.23428

R14 3.47654 -0.00034 0.00036 -0.11069 -0.03284 3.44369

R15 2.88104 0.00000 0.00007 -0.04194 -0.01252 2.86852

R16 2.06383 0.00008 0.00012 -0.05291 -0.01575 2.04808

R17 2.06036 -0.00005 0.00012 -0.05898 -0.01758 2.04279

R18 2.89434 -0.00006 0.00003 -0.03859 -0.01155 2.88279

R19 2.07243 -0.00001 0.00009 -0.04585 -0.01366 2.05877

R20 2.07097 0.00002 0.00009 -0.04000 -0.01191 2.05907

R21 2.88596 0.00003 0.00007 -0.03627 -0.01081 2.87515

R22 2.07208 -0.00001 0.00009 -0.04317 -0.01287 2.05922

R23 2.07179 0.00000 0.00006 -0.04129 -0.01232 2.05947

R24 2.06776 -0.00001 0.00010 -0.04417 -0.01315 2.05461

R25 2.06928 -0.00001 0.00008 -0.04622 -0.01378 2.05550

R26 2.06910 -0.00002 0.00009 -0.04426 -0.01319 2.05590

A1 2.17710 0.00015 -0.00033 0.06411 0.01594 2.19304

A2 1.97608 -0.00018 0.00006 -0.11637 -0.03778 1.93830

A3 2.12948 0.00003 0.00031 0.03791 0.00876 2.13824

A4 2.02335 0.00000 0.00006 -0.01148 -0.00334 2.02001

A5 1.83731 0.00005 -0.00140 0.08696 0.02473 1.86204

A6 1.87127 0.00008 -0.00033 0.07830 0.02321 1.89448

A7 1.94658 -0.00003 0.00040 -0.06711 -0.01982 1.92676

A8 1.94002 -0.00001 -0.00005 0.01902 0.00526 1.94527

A9 1.83256 -0.00009 0.00139 -0.10975 -0.03182 1.80075

A10 1.87347 -0.00012 0.00057 -0.08036 -0.02354 1.84993

A11 1.91159 0.00006 0.00023 0.01347 0.00426 1.91585

A12 1.92850 -0.00006 -0.00034 0.03893 0.01133 1.93984

A13 1.95242 -0.00002 0.00033 -0.02180 -0.00620 1.94622

A14 1.88379 -0.00002 0.00002 -0.02027 -0.00610 1.87768

A15 1.89332 0.00000 0.00010 -0.00318 -0.00085 1.89247

A16 1.89258 0.00003 -0.00034 -0.00814 -0.00277 1.88981

A17 1.79326 -0.00067 0.00106 -0.06169 -0.01745 1.77581

A18 1.97249 -0.00031 0.00088 -0.18834 -0.05690 1.91559

A19 2.14192 0.00011 -0.00002 0.02570 0.00646 2.14839

A20 2.15375 0.00010 -0.00080 0.11280 0.03166 2.18541

A21 1.79282 0.00047 -0.00004 0.09656 0.02893 1.82175

A22 1.92869 -0.00050 -0.00007 -0.05919 -0.01790 1.91079

A23 1.87451 0.00024 0.00014 0.05207 0.01585 1.89036

A24 1.89522 0.00008 -0.00014 -0.05040 -0.01538 1.87984

A25 1.93858 0.00012 0.00022 0.04094 0.01252 1.95110

A26 1.93833 0.00012 -0.00021 0.01036 0.00266 1.94100

A27 1.88652 -0.00004 0.00008 0.00696 0.00215 1.88867

A28 1.95240 0.00020 0.00024 0.01653 0.00516 1.95756

A29 1.91802 -0.00014 -0.00027 -0.03764 -0.01154 1.90648

A30 1.91525 0.00001 0.00014 0.03559 0.01078 1.92603

A31 1.90597 0.00001 -0.00002 0.01566 0.00470 1.91067

A32 1.91020 -0.00012 -0.00002 0.00256 0.00067 1.91087

A33 1.85965 0.00004 -0.00009 -0.03519 -0.01062 1.84903

A34 1.96731 -0.00015 -0.00007 -0.01692 -0.00519 1.96212

A35 1.90639 0.00003 0.00014 0.03553 0.01077 1.91717

A36 1.90681 0.00008 -0.00002 0.00204 0.00054 1.90735

A37 1.91275 0.00005 0.00001 0.03600 0.01080 1.92356

A38 1.91278 0.00002 0.00004 -0.02833 -0.00847 1.90431

A39 1.85435 -0.00002 -0.00011 -0.02897 -0.00876 1.84558

A40 1.94528 -0.00001 0.00021 0.00447 0.00155 1.94683

A41 1.94234 0.00000 0.00013 0.00992 0.00310 1.94543

A42 1.94360 -0.00006 -0.00012 0.02602 0.00768 1.95128

A43 1.87643 0.00001 -0.00013 -0.00491 -0.00160 1.87483

A44 1.87699 0.00003 -0.00018 -0.01547 -0.00482 1.87216

A45 1.87576 0.00003 0.00007 -0.02276 -0.00677 1.86899

D1 2.66798 0.00000 0.00394 -0.25732 -0.07326 2.59472

D2 -1.45514 0.00000 0.00342 -0.28465 -0.08208 -1.53722

D3 0.48975 -0.00005 0.00423 -0.33748 -0.09695 0.39280

D4 -0.50788 0.00006 0.00534 -0.72704 -0.21274 -0.72062

D5 1.65219 0.00006 0.00482 -0.75437 -0.22157 1.43062

D6 -2.68610 0.00001 0.00563 -0.80720 -0.23644 -2.92254

D7 -3.10399 -0.00006 -0.00064 0.24297 0.07183 -3.03216

D8 0.00440 -0.00001 0.00070 -0.21153 -0.06233 -0.05793

D9 -3.11993 -0.00002 -0.00271 0.10122 0.02763 -3.09230

D10 -1.04697 -0.00004 -0.00275 0.10840 0.02977 -1.01720

D11 1.06344 -0.00005 -0.00320 0.11024 0.02985 1.09329

D12 1.06117 -0.00007 -0.00120 0.04686 0.01284 1.07402

D13 3.13414 -0.00009 -0.00124 0.05404 0.01498 -3.13406

D14 -1.03864 -0.00010 -0.00169 0.05587 0.01507 -1.02357

D15 -0.97748 0.00007 -0.00316 0.21412 0.06108 -0.91639

D16 1.09549 0.00005 -0.00320 0.22130 0.06322 1.15871

D17 -3.07729 0.00004 -0.00364 0.22313 0.06331 -3.01398

D18 3.13233 0.00029 0.00642 1.74553 0.52996 -2.62089

D19 -0.94282 0.00030 0.00578 1.74908 0.53015 -0.41267

D20 1.16007 0.00022 0.00680 1.66797 0.50766 1.66773

D21 1.84777 -0.00031 0.00087 -0.39435 -0.11684 1.73093

D22 -1.11406 0.00025 0.00059 -0.10935 -0.03281 -1.14687

D23 2.54741 0.00028 -0.00061 0.98230 0.29434 2.84174

D24 -0.77535 -0.00028 -0.00024 0.68442 0.20483 -0.57052

D25 -2.99021 -0.00016 -0.00781 -1.61303 -0.49156 2.80141

D26 -0.87315 -0.00016 -0.00750 -1.56547 -0.47712 -1.35027

D27 1.16297 -0.00004 -0.00741 -1.55569 -0.47429 0.68868

D28 -3.10252 0.00001 0.00024 -0.23418 -0.07002 3.11064

D29 -0.98237 0.00006 0.00020 -0.22929 -0.06862 -1.05099

D30 1.05706 0.00003 0.00001 -0.27315 -0.08199 0.97506

D31 1.10203 -0.00004 -0.00002 -0.28711 -0.08610 1.01593

D32 -3.06100 0.00000 -0.00007 -0.28223 -0.08470 3.13748

D33 -1.02158 -0.00002 -0.00025 -0.32608 -0.09807 -1.11965

D34 -0.99807 -0.00015 -0.00012 -0.33036 -0.09921 -1.09728

D35 1.12208 -0.00010 -0.00017 -0.32547 -0.09781 1.02427

D36 -3.12167 -0.00013 -0.00036 -0.36932 -0.11118 3.05033

D37 -3.12583 -0.00004 0.00089 -0.65688 -0.19618 2.96117

D38 -0.99520 -0.00006 0.00096 -0.59701 -0.17813 -1.17333

D39 1.02638 -0.00001 0.00090 -0.61075 -0.18232 0.84406

D40 1.03026 0.00000 0.00108 -0.63102 -0.18824 0.84203

D41 -3.12228 -0.00002 0.00115 -0.57114 -0.17019 2.99071

D42 -1.10071 0.00003 0.00109 -0.58488 -0.17438 -1.27509

D43 -0.99933 0.00002 0.00121 -0.59907 -0.17852 -1.17785

D44 1.13131 0.00000 0.00128 -0.53919 -0.16047 0.97084

D45 -3.13030 0.00005 0.00122 -0.55293 -0.16466 2.98823

D46 -3.13840 -0.00003 0.00152 -0.14141 -0.04091 3.10388

D47 -1.04386 -0.00002 0.00159 -0.13788 -0.03979 -1.08365

D48 1.04869 -0.00002 0.00168 -0.14250 -0.04108 1.00761

D49 1.01774 0.00000 0.00138 -0.20109 -0.05896 0.95878

D50 3.11227 0.00001 0.00144 -0.19756 -0.05784 3.05443

D51 -1.07836 0.00001 0.00154 -0.20217 -0.05913 -1.13749

D52 -1.01079 -0.00002 0.00148 -0.17055 -0.04967 -1.06046

D53 1.08374 -0.00001 0.00154 -0.16702 -0.04854 1.03520

D54 -3.10690 -0.00001 0.00164 -0.17164 -0.04983 3.12646

Item Value Threshold Converged?

Maximum Force 0.000665 0.000450 NO

RMS Force 0.000137 0.000300 YES

Maximum Displacement 2.202095 0.001800 NO

RMS Displacement 0.626377 0.001200 NO

Predicted change in Energy=-7.564497D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:40:28 2019, MaxMem= 1342177280 cpu: 2.1

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -3.786750 -0.778220 0.018205

2 6 0 -2.765972 0.132916 0.589924

3 8 0 -4.890832 -0.472214 -0.293031

4 8 0 -3.248181 -1.958460 -0.309406

5 6 0 -1.783043 -0.501226 1.550294

6 16 0 -1.846578 0.913574 -0.879728

7 6 0 -0.256426 1.191176 -0.198875

8 16 0 0.861073 -0.128757 -0.703717

9 16 0 0.035251 2.298812 1.072865

10 6 0 2.525702 0.541859 -0.387253

11 6 0 3.524154 -0.598705 -0.307252

12 6 0 4.949291 -0.101435 -0.086182

13 6 0 5.913301 -1.231060 0.244707

14 1 0 -3.270532 0.974802 1.039839

15 1 0 -3.941257 -2.450121 -0.759755

16 1 0 -1.115834 0.256604 1.945862

17 1 0 -2.297019 -0.958530 2.392635

18 1 0 -1.186113 -1.262305 1.062704

19 1 0 2.770290 1.235560 -1.183223

20 1 0 2.486817 1.093492 0.541587

21 1 0 3.242092 -1.266182 0.506271

22 1 0 3.485825 -1.200302 -1.214921

23 1 0 5.292706 0.440740 -0.966830

24 1 0 4.955486 0.622895 0.728082

25 1 0 6.930737 -0.866163 0.362152

26 1 0 5.637784 -1.731088 1.170559

27 1 0 5.930189 -1.989300 -0.535290

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.482909 0.000000

3 O 1.187225 2.379248 0.000000

4 O 1.338041 2.327052 2.215287 0.000000

5 C 2.537492 1.513471 3.613453 2.780044 0.000000

6 S 2.726301 1.901208 3.395895 3.246280 2.812597

7 C 4.048313 2.835480 4.924780 4.345460 2.873044

8 S 4.748182 3.859720 5.776767 4.515447 3.494374

9 S 5.018777 3.573680 5.814684 5.551212 3.372587

10 C 6.461738 5.396659 7.486134 6.292486 4.838120

11 C 7.320346 6.395770 8.415948 6.907492 5.623728

12 C 8.762839 7.748376 9.849279 8.408146 6.939901

13 C 9.713257 8.792576 10.844091 9.207003 7.840341

14 H 2.093634 1.079711 2.548680 3.228775 2.156814

15 H 1.850500 3.142453 2.243131 0.961718 3.713813

16 H 3.452610 2.139351 4.449094 3.813089 1.084412

17 H 2.808866 2.158920 3.765259 3.034072 1.087583

18 H 2.844051 2.160119 4.023332 2.572827 1.083195

19 H 6.963728 5.916931 7.899476 6.869302 5.587610

20 H 6.567715 5.340116 7.587999 6.552007 4.668225

21 H 7.062644 6.169385 8.210586 6.577858 5.189136

22 H 7.388444 6.642282 8.458627 6.836782 5.991335

23 H 9.213722 8.213436 10.246557 8.895791 7.568979

24 H 8.882215 7.738223 9.959514 8.662559 6.880950

25 H 10.723366 9.750703 11.846264 10.259360 8.801979

26 H 9.542417 8.627558 10.704140 9.011235 7.531629

27 H 9.807751 9.021814 10.929535 9.181201 8.127607

6 7 8 9 10

6 S 0.000000

7 C 1.751916 0.000000

8 S 2.906684 1.801636 0.000000

9 S 3.045125 1.711507 3.119506 0.000000

10 C 4.415602 2.863099 1.822324 3.379524 0.000000

11 C 5.608875 4.184280 2.733136 4.740546 1.517956

12 C 6.916922 5.364982 4.134686 5.590382 2.525521

13 C 8.128932 6.643006 5.257337 6.906325 3.875364

14 H 2.390843 3.265895 4.618224 3.561221 5.985012

15 H 3.964407 5.210722 5.334252 6.459372 7.135284

16 H 2.991581 2.492370 3.328203 2.501546 4.334234

17 H 3.796845 3.937155 4.499941 4.218004 5.765206

18 H 2.990603 2.911266 2.931918 3.764756 4.374353

19 H 4.638023 3.183067 2.395077 3.701470 1.083795

20 H 4.564080 2.843098 2.384894 2.783026 1.080997

21 H 5.706742 4.333067 2.902940 4.828462 2.140237

22 H 5.745899 4.555871 2.880774 5.420722 2.154529

23 H 7.155455 5.652059 4.475815 5.937476 2.828859

24 H 6.995544 5.324117 4.402187 5.209251 2.674769

25 H 9.041626 7.496846 6.206502 7.620362 4.684919

26 H 8.198389 6.719872 5.375625 6.902030 4.156696

27 H 8.308034 6.964396 5.402400 7.464876 4.244904

11 12 13 14 15

11 C 0.000000

12 C 1.525505 0.000000

13 C 2.532303 1.521464 0.000000

14 H 7.103403 8.366105 9.478442 0.000000

15 H 7.704860 9.220189 9.980350 3.926641 0.000000

16 H 5.228533 6.406492 7.383483 2.445284 4.757073

17 H 6.426891 7.706372 8.491009 2.552559 3.855636

18 H 4.950127 6.349075 7.146453 3.057772 3.510425

19 H 2.167986 2.781924 4.242843 6.442168 7.668666

20 H 2.158732 2.808153 4.151201 5.780088 7.454584

21 H 1.089452 2.149922 2.684215 6.908037 7.389522

22 H 1.089611 2.150184 2.832684 7.447374 7.545249

23 H 2.154823 1.089691 2.155892 8.811412 9.678121

24 H 2.147774 1.089825 2.142010 8.239443 9.529383

25 H 3.482018 2.170700 1.087253 10.388181 11.043906

26 H 2.816673 2.170067 1.087723 9.311123 9.798017

27 H 2.788326 2.174372 1.087938 9.793886 9.884746

16 17 18 19 20

16 H 0.000000

17 H 1.752528 0.000000

18 H 1.758406 1.759292 0.000000

19 H 5.084436 6.578633 5.190052 0.000000

20 H 3.956193 5.524696 4.394514 1.753714 0.000000

21 H 4.835578 5.859588 4.463030 3.055438 2.477852

22 H 5.769609 6.820132 5.197925 2.538980 3.056931

23 H 7.041808 8.417119 6.999605 2.653516 3.251833

24 H 6.203071 7.607265 6.433133 2.967074 2.520034

25 H 8.277442 9.448962 8.156652 4.910677 4.860131

26 H 7.082610 8.065446 6.840830 4.750138 4.278136

27 H 7.800426 8.793304 7.329657 4.561195 4.745533

21 22 23 24 25

21 H 0.000000

22 H 1.739611 0.000000

23 H 3.047725 2.453443 0.000000

24 H 2.559987 3.042895 1.737706 0.000000

25 H 3.713070 3.803449 2.481398 2.500563 0.000000

26 H 2.529180 3.256251 3.066651 2.490492 1.753096

27 H 2.972140 2.656940 2.549060 3.060999 1.751552

26 27

26 H 0.000000

27 H 1.749885 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.46D-01

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -3.771009 -0.890202 0.198548

2 6 0 -2.757332 0.131747 0.555057

3 8 0 -4.874819 -0.668086 -0.177978

4 8 0 -3.225437 -2.110864 0.146715

5 6 0 -1.776579 -0.264935 1.637351

6 16 0 -1.833813 0.567335 -1.048678

7 6 0 -0.248494 0.999641 -0.441154

8 16 0 0.877545 -0.393746 -0.631940

9 16 0 0.031566 2.366297 0.550347

10 6 0 2.537469 0.340061 -0.467493

11 6 0 3.540610 -0.747803 -0.129187

12 6 0 4.962325 -0.205671 -0.019715

13 6 0 5.929669 -1.226697 0.560462

14 1 0 -3.268011 1.050381 0.802233

15 1 0 -3.913939 -2.694981 -0.184454

16 1 0 -1.114855 0.566089 1.855225

17 1 0 -2.292876 -0.524135 2.558812

18 1 0 -1.173700 -1.112780 1.335681

19 1 0 2.783079 0.838533 -1.397984

20 1 0 2.491264 1.086059 0.313473

21 1 0 3.257318 -1.216987 0.812364

22 1 0 3.509718 -1.538159 -0.878610

23 1 0 5.307882 0.126675 -0.998267

24 1 0 4.961020 0.683113 0.610983

25 1 0 6.944828 -0.839098 0.597047

26 1 0 5.651582 -1.507441 1.573868

27 1 0 5.954031 -2.140696 -0.029132

---------------------------------------------------------------------

Rotational constants (GHZ): 1.0764905 0.2210928 0.2015271

Leave Link 202 at Sat Aug 17 17:40:28 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1126.8878027117 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0569365337 Hartrees.

Nuclear repulsion after empirical dispersion term = 1126.8308661780 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2274

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.30D-10

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 98

GePol: Fraction of low-weight points (<1% of avg) = 4.31%

GePol: Cavity surface area = 300.350 Ang\*\*2

GePol: Cavity volume = 315.062 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0053275944 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1126.8255385836 Hartrees.

Leave Link 301 at Sat Aug 17 17:40:28 2019, MaxMem= 1342177280 cpu: 0.8

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.84D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 299 299 299 299 299 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:40:28 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:40:28 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999869 -0.004862 -0.010675 -0.011115 Ang= -1.85 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7554 S= 0.5027

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.63325027582

Leave Link 401 at Sat Aug 17 17:40:29 2019, MaxMem= 1342177280 cpu: 7.7

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 750000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 15513228.

Iteration 1 A\*A^-1 deviation from unit magnitude is 4.77D-15 for 856.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.80D-15 for 536 251.

Iteration 1 A^-1\*A deviation from unit magnitude is 4.88D-15 for 2261.

Iteration 1 A^-1\*A deviation from orthogonality is 1.11D-12 for 976 975.

E= -1657.96744428955

DIIS: error= 2.40D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1657.96744428955 IErMin= 1 ErrMin= 2.40D-02

ErrMax= 2.40D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.61D+00 BMatP= 1.61D+00

IDIUse=3 WtCom= 7.60D-01 WtEn= 2.40D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Recover alternate guess density for next cycle.

RMSDP=3.90D-03 MaxDP=9.82D-02 OVMax= 0.00D+00

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.86D-03 CP: 9.66D-01

E= -1658.19921664629 Delta-E= -0.231772356738 Rises=F Damp=F

DIIS: error= 3.54D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.19921664629 IErMin= 1 ErrMin= 2.40D-02

ErrMax= 3.54D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.25D+00 BMatP= 1.61D+00

IDIUse=2 WtCom= 0.00D+00 WtEn= 1.00D+00

Coeff-En: 0.000D+00 0.100D+01

Coeff: 0.000D+00 0.100D+01

Gap= 0.128 Goal= None Shift= 0.000

Gap= 0.160 Goal= None Shift= 0.000

RMSDP=4.58D-03 MaxDP=1.91D-01 DE=-2.32D-01 OVMax= 2.15D-01

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.91D-03 CP: 9.67D-01 3.83D-01

E= -1657.86959868099 Delta-E= 0.329617965296 Rises=F Damp=F

DIIS: error= 4.11D-02 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1658.19921664629 IErMin= 1 ErrMin= 2.40D-02

ErrMax= 4.11D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.50D+00 BMatP= 1.61D+00

IDIUse=2 WtCom= 0.00D+00 WtEn= 1.00D+00

Coeff-En: 0.000D+00 0.621D+00 0.379D+00

Coeff: 0.000D+00 0.621D+00 0.379D+00

Gap= 0.144 Goal= None Shift= 0.000

Gap= 0.215 Goal= None Shift= 0.000

RMSDP=2.60D-03 MaxDP=1.20D-01 DE= 3.30D-01 OVMax= 1.24D-01

Cycle 4 Pass 1 IDiag 1:

RMSU= 8.44D-04 CP: 9.66D-01 6.71D-01 4.37D-01

E= -1658.65016206268 Delta-E= -0.780563381686 Rises=F Damp=F

DIIS: error= 5.68D-03 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.65016206268 IErMin= 4 ErrMin= 5.68D-03

ErrMax= 5.68D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.13D-02 BMatP= 1.61D+00

IDIUse=3 WtCom= 9.43D-01 WtEn= 5.68D-02

Coeff-Com: 0.125D-01 0.202D+00 0.114D+00 0.672D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.100D+01

Coeff: 0.118D-01 0.191D+00 0.107D+00 0.690D+00

Gap= 0.116 Goal= None Shift= 0.000

Gap= 0.138 Goal= None Shift= 0.000

RMSDP=5.62D-04 MaxDP=1.98D-02 DE=-7.81D-01 OVMax= 4.73D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.52D-04 CP: 9.68D-01 7.02D-01 3.97D-01 6.82D-01

E= -1658.65614592586 Delta-E= -0.005983863182 Rises=F Damp=F

DIIS: error= 6.94D-03 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.65614592586 IErMin= 4 ErrMin= 5.68D-03

ErrMax= 6.94D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.14D-02 BMatP= 7.13D-02

IDIUse=3 WtCom= 9.31D-01 WtEn= 6.94D-02

Coeff-Com: -0.120D-02 0.338D-01-0.659D-02 0.486D+00 0.488D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.399D+00 0.601D+00

Coeff: -0.112D-02 0.315D-01-0.614D-02 0.480D+00 0.496D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.137 Goal= None Shift= 0.000

RMSDP=3.32D-04 MaxDP=1.73D-02 DE=-5.98D-03 OVMax= 3.42D-02

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.86D-04 CP: 9.66D-01 6.94D-01 3.96D-01 8.54D-01 4.92D-01

E= -1658.66635564384 Delta-E= -0.010209717986 Rises=F Damp=F

DIIS: error= 1.06D-03 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.66635564384 IErMin= 6 ErrMin= 1.06D-03

ErrMax= 1.06D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.42D-03 BMatP= 5.14D-02

IDIUse=3 WtCom= 9.89D-01 WtEn= 1.06D-02

Coeff-Com: 0.236D-03 0.552D-02-0.854D-02 0.190D+00 0.242D+00 0.571D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.100D+01

Coeff: 0.233D-03 0.546D-02-0.845D-02 0.188D+00 0.239D+00 0.575D+00

Gap= 0.124 Goal= None Shift= 0.000

Gap= 0.138 Goal= None Shift= 0.000

RMSDP=6.94D-05 MaxDP=3.02D-03 DE=-1.02D-02 OVMax= 6.20D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.13D-05 CP: 9.66D-01 6.91D-01 3.95D-01 8.84D-01 5.59D-01

CP: 8.75D-01

E= -1658.66666071957 Delta-E= -0.000305075725 Rises=F Damp=F

DIIS: error= 2.79D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.66666071957 IErMin= 7 ErrMin= 2.79D-04

ErrMax= 2.79D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.23D-04 BMatP= 1.42D-03

IDIUse=3 WtCom= 9.97D-01 WtEn= 2.79D-03

Coeff-Com: -0.197D-03-0.142D-02-0.393D-02 0.313D-01 0.514D-01 0.252D+00

Coeff-Com: 0.671D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00

Coeff-En: 0.100D+01

Coeff: -0.197D-03-0.142D-02-0.392D-02 0.312D-01 0.512D-01 0.251D+00

Coeff: 0.672D+00

Gap= 0.124 Goal= None Shift= 0.000

Gap= 0.138 Goal= None Shift= 0.000

RMSDP=2.69D-05 MaxDP=1.08D-03 DE=-3.05D-04 OVMax= 3.78D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.87D-05 CP: 9.66D-01 6.91D-01 3.94D-01 8.97D-01 5.70D-01

CP: 9.49D-01 1.07D+00

E= -1658.66669966396 Delta-E= -0.000038944391 Rises=F Damp=F

DIIS: error= 7.67D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.66669966396 IErMin= 8 ErrMin= 7.67D-05

ErrMax= 7.67D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.72D-05 BMatP= 1.23D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.417D-04-0.125D-02-0.914D-03-0.781D-02-0.561D-02 0.282D-01

Coeff-Com: 0.246D+00 0.742D+00

Coeff: 0.417D-04-0.125D-02-0.914D-03-0.781D-02-0.561D-02 0.282D-01

Coeff: 0.246D+00 0.742D+00

Gap= 0.124 Goal= None Shift= 0.000

Gap= 0.138 Goal= None Shift= 0.000

RMSDP=2.28D-05 MaxDP=9.20D-04 DE=-3.89D-05 OVMax= 3.91D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.05D-05 CP: 9.66D-01 6.90D-01 3.93D-01 9.05D-01 5.69D-01

CP: 1.03D+00 1.27D+00 1.08D+00

E= -1658.66670761509 Delta-E= -0.000007951129 Rises=F Damp=F

DIIS: error= 7.22D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.66670761509 IErMin= 9 ErrMin= 7.22D-05

ErrMax= 7.22D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.59D-06 BMatP= 1.72D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.576D-04-0.414D-03 0.808D-03-0.180D-01-0.228D-01-0.678D-01

Coeff-Com: -0.672D-01 0.483D+00 0.693D+00

Coeff: 0.576D-04-0.414D-03 0.808D-03-0.180D-01-0.228D-01-0.678D-01

Coeff: -0.672D-01 0.483D+00 0.693D+00

Gap= 0.124 Goal= None Shift= 0.000

Gap= 0.138 Goal= None Shift= 0.000

RMSDP=1.14D-05 MaxDP=6.46D-04 DE=-7.95D-06 OVMax= 1.92D-03

Cycle 10 Pass 1 IDiag 1:

RMSU= 4.91D-06 CP: 9.66D-01 6.90D-01 3.92D-01 9.10D-01 5.75D-01

CP: 1.06D+00 1.37D+00 1.32D+00 7.68D-01

E= -1658.66671153227 Delta-E= -0.000003917183 Rises=F Damp=F

DIIS: error= 3.05D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.66671153227 IErMin=10 ErrMin= 3.05D-05

ErrMax= 3.05D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.68D-06 BMatP= 9.59D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.134D-05 0.211D-04 0.768D-03-0.101D-01-0.135D-01-0.498D-01

Coeff-Com: -0.932D-01 0.146D+00 0.456D+00 0.563D+00

Coeff: 0.134D-05 0.211D-04 0.768D-03-0.101D-01-0.135D-01-0.498D-01

Coeff: -0.932D-01 0.146D+00 0.456D+00 0.563D+00

Gap= 0.124 Goal= None Shift= 0.000

Gap= 0.138 Goal= None Shift= 0.000

RMSDP=5.46D-06 MaxDP=2.43D-04 DE=-3.92D-06 OVMax= 9.03D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.73D-06 CP: 9.66D-01 6.90D-01 3.92D-01 9.12D-01 5.76D-01

CP: 1.07D+00 1.42D+00 1.42D+00 9.84D-01 8.39D-01

E= -1658.66671231569 Delta-E= -0.000000783420 Rises=F Damp=F

DIIS: error= 7.78D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.66671231569 IErMin=11 ErrMin= 7.78D-06

ErrMax= 7.78D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.33D-07 BMatP= 2.68D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.122D-04 0.465D-04 0.202D-03-0.152D-02-0.216D-02-0.106D-01

Coeff-Com: -0.272D-01-0.548D-02 0.108D+00 0.207D+00 0.732D+00

Coeff: 0.122D-04 0.465D-04 0.202D-03-0.152D-02-0.216D-02-0.106D-01

Coeff: -0.272D-01-0.548D-02 0.108D+00 0.207D+00 0.732D+00

Gap= 0.124 Goal= None Shift= 0.000

Gap= 0.138 Goal= None Shift= 0.000

RMSDP=1.08D-06 MaxDP=6.90D-05 DE=-7.83D-07 OVMax= 2.02D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 7.49D-07 CP: 9.66D-01 6.90D-01 3.92D-01 9.12D-01 5.76D-01

CP: 1.07D+00 1.42D+00 1.44D+00 1.01D+00 9.47D-01

CP: 9.61D-01

E= -1658.66671235883 Delta-E= -0.000000043135 Rises=F Damp=F

DIIS: error= 4.37D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.66671235883 IErMin=12 ErrMin= 4.37D-06

ErrMax= 4.37D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.63D-08 BMatP= 1.33D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.325D-05 0.206D-04-0.285D-04 0.973D-03 0.114D-02 0.303D-02

Coeff-Com: 0.296D-02-0.286D-01-0.263D-01-0.152D-01 0.392D+00 0.670D+00

Coeff: -0.325D-05 0.206D-04-0.285D-04 0.973D-03 0.114D-02 0.303D-02

Coeff: 0.296D-02-0.286D-01-0.263D-01-0.152D-01 0.392D+00 0.670D+00

Gap= 0.124 Goal= None Shift= 0.000

Gap= 0.138 Goal= None Shift= 0.000

RMSDP=5.67D-07 MaxDP=2.93D-05 DE=-4.31D-08 OVMax= 6.27D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 3.04D-07 CP: 9.66D-01 6.90D-01 3.92D-01 9.12D-01 5.76D-01

CP: 1.07D+00 1.43D+00 1.44D+00 1.04D+00 9.81D-01

CP: 1.14D+00 9.22D-01

E= -1658.66671237286 Delta-E= -0.000000014031 Rises=F Damp=F

DIIS: error= 1.79D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1658.66671237286 IErMin=13 ErrMin= 1.79D-06

ErrMax= 1.79D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.51D-09 BMatP= 4.63D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.261D-06 0.419D-05-0.522D-04 0.714D-03 0.869D-03 0.332D-02

Coeff-Com: 0.645D-02-0.108D-01-0.291D-01-0.451D-01 0.520D-01 0.281D+00

Coeff-Com: 0.741D+00

Coeff: -0.261D-06 0.419D-05-0.522D-04 0.714D-03 0.869D-03 0.332D-02

Coeff: 0.645D-02-0.108D-01-0.291D-01-0.451D-01 0.520D-01 0.281D+00

Coeff: 0.741D+00

Gap= 0.124 Goal= None Shift= 0.000

Gap= 0.138 Goal= None Shift= 0.000

RMSDP=2.25D-07 MaxDP=1.14D-05 DE=-1.40D-08 OVMax= 3.75D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 1.14D-07 CP: 9.66D-01 6.90D-01 3.92D-01 9.12D-01 5.76D-01

CP: 1.07D+00 1.43D+00 1.44D+00 1.04D+00 9.99D-01

CP: 1.21D+00 1.07D+00 9.15D-01

E= -1658.66671237455 Delta-E= -0.000000001689 Rises=F Damp=F

DIIS: error= 3.64D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1658.66671237455 IErMin=14 ErrMin= 3.64D-07

ErrMax= 3.64D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.23D-10 BMatP= 4.51D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.222D-06-0.110D-05-0.115D-04 0.628D-04 0.718D-04 0.478D-03

Coeff-Com: 0.104D-02 0.385D-03-0.323D-02-0.968D-02-0.354D-01-0.159D-01

Coeff-Com: 0.231D+00 0.831D+00

Coeff: -0.222D-06-0.110D-05-0.115D-04 0.628D-04 0.718D-04 0.478D-03

Coeff: 0.104D-02 0.385D-03-0.323D-02-0.968D-02-0.354D-01-0.159D-01

Coeff: 0.231D+00 0.831D+00

Gap= 0.124 Goal= None Shift= 0.000

Gap= 0.138 Goal= None Shift= 0.000

RMSDP=8.03D-08 MaxDP=3.83D-06 DE=-1.69D-09 OVMax= 1.52D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 3.93D-08 CP: 9.66D-01 6.90D-01 3.92D-01 9.12D-01 5.76D-01

CP: 1.07D+00 1.43D+00 1.44D+00 1.04D+00 1.00D+00

CP: 1.23D+00 1.11D+00 1.06D+00 9.26D-01

E= -1658.66671237472 Delta-E= -0.000000000171 Rises=F Damp=F

DIIS: error= 1.84D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1658.66671237472 IErMin=15 ErrMin= 1.84D-07

ErrMax= 1.84D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.03D-11 BMatP= 4.23D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.499D-08-0.102D-05 0.137D-06-0.426D-04-0.523D-04-0.104D-03

Coeff-Com: -0.185D-03 0.107D-02 0.153D-02 0.248D-06-0.199D-01-0.347D-01

Coeff-Com: 0.288D-01 0.354D+00 0.669D+00

Coeff: 0.499D-08-0.102D-05 0.137D-06-0.426D-04-0.523D-04-0.104D-03

Coeff: -0.185D-03 0.107D-02 0.153D-02 0.248D-06-0.199D-01-0.347D-01

Coeff: 0.288D-01 0.354D+00 0.669D+00

Gap= 0.124 Goal= None Shift= 0.000

Gap= 0.138 Goal= None Shift= 0.000

RMSDP=2.16D-08 MaxDP=1.07D-06 DE=-1.71D-10 OVMax= 2.26D-06

Cycle 16 Pass 1 IDiag 1:

RMSU= 1.19D-08 CP: 9.66D-01 6.90D-01 3.92D-01 9.12D-01 5.76D-01

CP: 1.07D+00 1.43D+00 1.44D+00 1.04D+00 1.00D+00

CP: 1.23D+00 1.11D+00 1.09D+00 1.02D+00 9.31D-01

E= -1658.66671237473 Delta-E= -0.000000000011 Rises=F Damp=F

DIIS: error= 5.54D-08 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1658.66671237473 IErMin=16 ErrMin= 5.54D-08

ErrMax= 5.54D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.46D-12 BMatP= 6.03D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.369D-07-0.306D-06 0.134D-05-0.196D-04-0.228D-04-0.823D-04

Coeff-Com: -0.174D-03 0.292D-03 0.898D-03 0.961D-03-0.247D-02-0.105D-01

Coeff-Com: -0.171D-01 0.328D-01 0.249D+00 0.746D+00

Coeff: 0.369D-07-0.306D-06 0.134D-05-0.196D-04-0.228D-04-0.823D-04

Coeff: -0.174D-03 0.292D-03 0.898D-03 0.961D-03-0.247D-02-0.105D-01

Coeff: -0.171D-01 0.328D-01 0.249D+00 0.746D+00

Gap= 0.124 Goal= None Shift= 0.000

Gap= 0.138 Goal= None Shift= 0.000

RMSDP=7.62D-09 MaxDP=3.53D-07 DE=-1.09D-11 OVMax= 1.41D-06

Error on total polarization charges = 0.04091

SCF Done: E(UB3LYP) = -1658.66671237 A.U. after 16 cycles

NFock= 16 Conv=0.76D-08 -V/T= 2.0018

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7551 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655701145534D+03 PE=-6.196935666917D+03 EE= 1.755742270424D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.34

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7551, after 0.7500

Leave Link 502 at Sat Aug 17 17:41:03 2019, MaxMem= 1342177280 cpu: 400.6

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 323

Leave Link 701 at Sat Aug 17 17:41:04 2019, MaxMem= 1342177280 cpu: 10.2

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:41:04 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:41:07 2019, MaxMem= 1342177280 cpu: 38.2

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.83030708D+00-3.17399030D+00 5.90865808D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.040238774 0.002444848 -0.006340312

2 6 0.003663673 0.006737237 0.010736873

3 8 -0.043223146 0.009666573 -0.005088340

4 8 0.003464314 -0.013377777 0.004517223

5 6 -0.002084505 -0.002179476 0.002080017

6 16 0.001239778 0.002041880 -0.003559887

7 6 0.000917375 -0.002884390 -0.007546958

8 16 -0.003141593 0.000929379 0.001100512

9 16 0.005131507 0.007853229 0.000582642

10 6 -0.001682164 -0.004079933 -0.002113407

11 6 0.002066030 0.001988550 0.000202199

12 6 -0.000082738 -0.001830374 0.001488342

13 6 0.000907159 0.000650190 -0.001252552

14 1 -0.004866259 0.001850872 0.005772339

15 1 -0.005189977 -0.008169090 -0.005207626

16 1 0.000832461 -0.000404874 0.001130676

17 1 -0.004650816 -0.002302716 0.002611048

18 1 0.001618071 -0.003250532 -0.000955367

19 1 0.002820721 0.003984974 -0.004056097

20 1 -0.000513108 0.002962147 0.005741400

21 1 -0.001073288 -0.001790941 0.003790500

22 1 0.000349344 -0.002217416 -0.004067007

23 1 0.001130670 0.001392036 -0.003956261

24 1 -0.000320979 0.002798960 0.003679141

25 1 0.004418927 0.001693643 0.000634005

26 1 -0.001688487 -0.001585115 0.004147753

27 1 -0.000281744 -0.002921885 -0.004070855

-------------------------------------------------------------------

Cartesian Forces: Max 0.043223146 RMS 0.007651244

Leave Link 716 at Sat Aug 17 17:41:08 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.049887921 RMS 0.007610391

Search for a local minimum.

Step number 25 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .76104D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 25 19

DE= 1.03D-02 DEPred=-7.56D-04 R=-1.36D+01

Trust test=-1.36D+01 RLast= 1.50D+00 DXMaxT set to 5.00D-02

ITU= -1 0 0 -1 1 -1 1 -1 1 1 -1 1 -1 1 1 -1 0 0 -1 0

ITU= 0 -1 -1 0 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.96245.

Iteration 1 RMS(Cart)= 0.36123175 RMS(Int)= 0.07509317

Iteration 2 RMS(Cart)= 0.21753580 RMS(Int)= 0.02838291

Iteration 3 RMS(Cart)= 0.08635922 RMS(Int)= 0.00291275

Iteration 4 RMS(Cart)= 0.00623609 RMS(Int)= 0.00001969

Iteration 5 RMS(Cart)= 0.00002436 RMS(Int)= 0.00001848

Iteration 6 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001848

ITry= 1 IFail=0 DXMaxC= 2.16D+00 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=T

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.80229 0.01372 0.03402 0.00000 0.03402 2.83631

R2 2.24353 0.04402 0.04300 0.00000 0.04300 2.28653

R3 2.52853 0.01849 0.02380 0.00000 0.02380 2.55233

R4 2.86005 0.00374 0.00637 0.00000 0.00637 2.86641

R5 3.59276 0.01581 0.00400 0.00000 0.00400 3.59676

R6 2.04036 0.00612 0.01710 0.00000 0.01710 2.05746

R7 1.81738 0.01036 0.01891 0.00000 0.01891 1.83630

R8 2.04924 0.00064 0.01178 0.00000 0.01178 2.06102

R9 2.05523 0.00519 0.01307 0.00000 0.01307 2.06830

R10 2.04694 0.00361 0.01292 0.00000 0.01292 2.05987

R11 3.31064 0.00701 0.00937 0.00000 0.00937 3.32001

R12 3.40460 -0.00003 -0.01990 0.00000 -0.01990 3.38470

R13 3.23428 0.00639 0.01916 0.00000 0.01916 3.25344

R14 3.44369 0.00595 0.03155 0.00000 0.03155 3.47524

R15 2.86852 0.00494 0.01203 0.00000 0.01203 2.88056

R16 2.04808 0.00617 0.01514 0.00000 0.01514 2.06322

R17 2.04279 0.00647 0.01689 0.00000 0.01689 2.05968

R18 2.88279 0.00398 0.01111 0.00000 0.01111 2.89390

R19 2.05877 0.00420 0.01313 0.00000 0.01313 2.07190

R20 2.05907 0.00460 0.01144 0.00000 0.01144 2.07051

R21 2.87515 0.00360 0.01039 0.00000 0.01039 2.88554

R22 2.05922 0.00425 0.01237 0.00000 0.01237 2.07159

R23 2.05947 0.00461 0.01185 0.00000 0.01185 2.07132

R24 2.05461 0.00477 0.01264 0.00000 0.01264 2.06725

R25 2.05550 0.00468 0.01325 0.00000 0.01325 2.06875

R26 2.05590 0.00495 0.01268 0.00000 0.01268 2.06859

A1 2.19304 -0.00480 -0.01528 0.00000 -0.01517 2.17786

A2 1.93830 0.01048 0.03635 0.00000 0.03645 1.97476

A3 2.13824 -0.00435 -0.00849 0.00000 -0.00838 2.12986

A4 2.02001 -0.00670 0.00320 0.00000 0.00320 2.02321

A5 1.86204 -0.00915 -0.02356 0.00000 -0.02356 1.83848

A6 1.89448 0.00168 -0.02228 0.00000 -0.02228 1.87220

A7 1.92676 0.01644 0.01901 0.00000 0.01901 1.94577

A8 1.94527 -0.00060 -0.00505 0.00000 -0.00504 1.94024

A9 1.80075 -0.00145 0.03038 0.00000 0.03039 1.83113

A10 1.84993 0.00669 0.02256 0.00000 0.02256 1.87249

A11 1.91585 0.00266 -0.00414 0.00000 -0.00414 1.91171

A12 1.93984 -0.00428 -0.01085 0.00000 -0.01085 1.92899

A13 1.94622 0.00101 0.00591 0.00000 0.00591 1.95213

A14 1.87768 0.00077 0.00587 0.00000 0.00587 1.88356

A15 1.89247 -0.00073 0.00081 0.00000 0.00080 1.89328

A16 1.88981 0.00060 0.00272 0.00000 0.00272 1.89254

A17 1.77581 0.04989 0.01661 0.00000 0.01661 1.79242

A18 1.91559 0.00603 0.05461 0.00000 0.05466 1.97025

A19 2.14839 0.00275 -0.00622 0.00000 -0.00617 2.14222

A20 2.18541 -0.00538 -0.03033 0.00000 -0.03029 2.15512

A21 1.82175 -0.00086 -0.02783 0.00000 -0.02783 1.79391

A22 1.91079 0.00456 0.01724 0.00000 0.01724 1.92803

A23 1.89036 -0.00034 -0.01528 0.00000 -0.01528 1.87508

A24 1.87984 -0.00188 0.01483 0.00000 0.01483 1.89467

A25 1.95110 -0.00260 -0.01208 0.00000 -0.01208 1.93901

A26 1.94100 -0.00042 -0.00253 0.00000 -0.00252 1.93848

A27 1.88867 0.00064 -0.00208 0.00000 -0.00208 1.88659

A28 1.95756 0.00092 -0.00501 0.00000 -0.00501 1.95255

A29 1.90648 -0.00017 0.01116 0.00000 0.01116 1.91763

A30 1.92603 -0.00041 -0.01040 0.00000 -0.01040 1.91563

A31 1.91067 -0.00024 -0.00452 0.00000 -0.00452 1.90615

A32 1.91087 -0.00067 -0.00064 0.00000 -0.00064 1.91023

A33 1.84903 0.00055 0.01023 0.00000 0.01023 1.85927

A34 1.96212 0.00159 0.00501 0.00000 0.00501 1.96713

A35 1.91717 -0.00067 -0.01039 0.00000 -0.01039 1.90677

A36 1.90735 -0.00066 -0.00051 0.00000 -0.00051 1.90684

A37 1.92356 -0.00104 -0.01040 0.00000 -0.01040 1.91316

A38 1.90431 0.00012 0.00814 0.00000 0.00814 1.91246

A39 1.84558 0.00060 0.00845 0.00000 0.00845 1.85404

A40 1.94683 0.00023 -0.00153 0.00000 -0.00153 1.94530

A41 1.94543 -0.00087 -0.00300 0.00000 -0.00300 1.94243

A42 1.95128 -0.00092 -0.00737 0.00000 -0.00737 1.94391

A43 1.87483 0.00034 0.00157 0.00000 0.00157 1.87639

A44 1.87216 0.00041 0.00467 0.00000 0.00467 1.87684

A45 1.86899 0.00093 0.00650 0.00000 0.00650 1.87549

D1 2.59472 -0.00808 0.06981 0.00000 0.06981 2.66453

D2 -1.53722 0.00169 0.07839 0.00000 0.07840 -1.45882

D3 0.39280 -0.00354 0.09256 0.00000 0.09256 0.48536

D4 -0.72062 0.00013 0.20381 0.00000 0.20382 -0.51680

D5 1.43062 0.00989 0.21240 0.00000 0.21240 1.64303

D6 -2.92254 0.00467 0.22656 0.00000 0.22656 -2.69597

D7 -3.03216 -0.00397 -0.06902 0.00000 -0.06900 -3.10116

D8 -0.05793 0.00381 0.05987 0.00000 0.05985 0.00193

D9 -3.09230 0.00044 -0.02611 0.00000 -0.02611 -3.11841

D10 -1.01720 0.00043 -0.02816 0.00000 -0.02816 -1.04536

D11 1.09329 -0.00106 -0.02817 0.00000 -0.02816 1.06513

D12 1.07402 0.00448 -0.01215 0.00000 -0.01215 1.06187

D13 -3.13406 0.00447 -0.01420 0.00000 -0.01420 3.13492

D14 -1.02357 0.00297 -0.01420 0.00000 -0.01420 -1.03778

D15 -0.91639 -0.00320 -0.05823 0.00000 -0.05823 -0.97463

D16 1.15871 -0.00321 -0.06029 0.00000 -0.06029 1.09842

D17 -3.01398 -0.00470 -0.06029 0.00000 -0.06029 -3.07427

D18 -2.62089 -0.00504 -0.51120 0.00000 -0.51119 -3.13209

D19 -0.41267 -0.00901 -0.51126 0.00000 -0.51125 -0.92392

D20 1.66773 -0.00269 -0.48980 0.00000 -0.48981 1.17792

D21 1.73093 0.00031 0.11230 0.00000 0.11228 1.84321

D22 -1.14687 -0.01181 0.03148 0.00000 0.03149 -1.11538

D23 2.84174 -0.00774 -0.28318 0.00000 -0.28319 2.55856

D24 -0.57052 0.00627 -0.19710 0.00000 -0.19709 -0.76761

D25 2.80141 0.00140 0.47448 0.00000 0.47448 -3.00730

D26 -1.35027 0.00080 0.46053 0.00000 0.46052 -0.88974

D27 0.68868 0.00038 0.45778 0.00000 0.45779 1.14647

D28 3.11064 -0.00012 0.06734 0.00000 0.06734 -3.10520

D29 -1.05099 0.00006 0.06601 0.00000 0.06601 -0.98498

D30 0.97506 0.00040 0.07891 0.00000 0.07892 1.05398

D31 1.01593 -0.00107 0.08287 0.00000 0.08287 1.09880

D32 3.13748 -0.00089 0.08153 0.00000 0.08153 -3.06417

D33 -1.11965 -0.00055 0.09444 0.00000 0.09444 -1.02521

D34 -1.09728 0.00020 0.09550 0.00000 0.09550 -1.00177

D35 1.02427 0.00039 0.09417 0.00000 0.09417 1.11844

D36 3.05033 0.00072 0.10707 0.00000 0.10707 -3.12578

D37 2.96117 0.00104 0.18866 0.00000 0.18866 -3.13336

D38 -1.17333 0.00033 0.17128 0.00000 0.17128 -1.00205

D39 0.84406 0.00030 0.17532 0.00000 0.17532 1.01937

D40 0.84203 0.00082 0.18098 0.00000 0.18098 1.02301

D41 2.99071 0.00010 0.16360 0.00000 0.16360 -3.12888

D42 -1.27509 0.00007 0.16764 0.00000 0.16764 -1.10745

D43 -1.17785 0.00066 0.17160 0.00000 0.17160 -1.00625

D44 0.97084 -0.00005 0.15422 0.00000 0.15422 1.12506

D45 2.98823 -0.00008 0.15826 0.00000 0.15826 -3.13670

D46 3.10388 -0.00020 0.03911 0.00000 0.03911 -3.14020

D47 -1.08365 -0.00021 0.03801 0.00000 0.03801 -1.04564

D48 1.00761 -0.00024 0.03924 0.00000 0.03924 1.04685

D49 0.95878 0.00030 0.05651 0.00000 0.05651 1.01528

D50 3.05443 0.00029 0.05541 0.00000 0.05541 3.10985

D51 -1.13749 0.00026 0.05664 0.00000 0.05664 -1.08085

D52 -1.06046 0.00009 0.04754 0.00000 0.04754 -1.01292

D53 1.03520 0.00008 0.04645 0.00000 0.04645 1.08164

D54 3.12646 0.00005 0.04767 0.00000 0.04767 -3.10906

Item Value Threshold Converged?

Maximum Force 0.049888 0.000450 NO

RMS Force 0.007610 0.000300 NO

Maximum Displacement 2.156205 0.001800 NO

RMS Displacement 0.606146 0.001200 NO

Predicted change in Energy=-4.521402D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:41:08 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.105433 -0.419177 -0.194585

2 6 0 -2.839926 0.064613 0.451305

3 8 0 -4.900322 0.288022 -0.770841

4 8 0 -4.262870 -1.758344 -0.116707

5 6 0 -2.330132 -0.764759 1.614514

6 16 0 -1.559882 0.154801 -0.954395

7 6 0 -0.113526 0.708236 -0.124713

8 16 0 1.099122 -0.590197 0.102476

9 16 0 -0.007926 2.249799 0.634560

10 6 0 2.694324 0.315667 -0.026852

11 6 0 3.862933 -0.662872 -0.046364

12 6 0 5.211692 0.060248 -0.101907

13 6 0 6.396088 -0.902979 -0.133798

14 1 0 -3.003614 1.099274 0.748096

15 1 0 -5.082272 -1.980705 -0.589347

16 1 0 -1.424867 -0.309479 2.017899

17 1 0 -3.074884 -0.800554 2.415756

18 1 0 -2.098353 -1.786435 1.313466

19 1 0 2.661375 0.906803 -0.944193

20 1 0 2.772487 1.002512 0.815822

21 1 0 3.831143 -1.299193 0.845927

22 1 0 3.771701 -1.331578 -0.909495

23 1 0 5.239064 0.706612 -0.986890

24 1 0 5.301708 0.724401 0.765401

25 1 0 7.348114 -0.365482 -0.171871

26 1 0 6.413516 -1.541197 0.755480

27 1 0 6.352901 -1.559674 -1.008522

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.500911 0.000000

3 O 1.209980 2.405990 0.000000

4 O 1.350636 2.381298 2.240949 0.000000

5 C 2.558117 1.516840 3.661168 2.778456 0.000000

6 S 2.717829 1.903324 3.348131 3.415844 2.835167

7 C 4.148646 2.859949 4.848451 4.827126 3.179303

8 S 5.215830 4.008311 6.125952 5.492137 3.751868

9 S 4.959888 3.581739 5.455205 5.893570 3.929442

10 C 6.841406 5.560539 7.631051 7.260314 5.395050

11 C 7.973469 6.760564 8.844416 8.199615 6.412718

12 C 9.329912 8.070602 10.136675 9.647529 7.778550

13 C 10.512835 9.304974 11.376871 10.693238 8.900709

14 H 2.099606 1.088762 2.561796 3.240307 2.163071

15 H 1.883725 3.208488 2.283237 0.971726 3.729585

16 H 3.477435 2.143957 4.495872 3.835364 1.090644

17 H 2.832200 2.159348 3.830356 2.956695 1.094498

18 H 2.858668 2.172471 4.061864 2.594479 1.090034

19 H 6.936125 5.737684 7.588953 7.465448 5.852884

20 H 7.095626 5.701904 7.867655 7.614997 5.458743

21 H 8.052722 6.820474 9.020625 8.163978 6.231987

22 H 7.961960 6.893094 8.823056 8.084861 6.627539

23 H 9.445357 8.231079 10.150322 9.854947 8.137873

24 H 9.524896 8.174362 10.326272 9.920852 7.821993

25 H 11.453695 10.216139 12.280473 11.694360 9.849824

26 H 10.621197 9.396666 11.561947 10.714153 8.819987

27 H 10.551776 9.448676 11.406380 10.655017 9.105343

6 7 8 9 10

6 S 0.000000

7 C 1.756875 0.000000

8 S 2.956738 1.791106 0.000000

9 S 3.053255 1.721646 3.094228 0.000000

10 C 4.357119 2.836849 1.839018 3.388287 0.000000

11 C 5.558779 4.206935 2.768769 4.891918 1.524325

12 C 6.825678 5.364546 4.168703 5.707971 2.531405

13 C 8.067821 6.706055 5.311451 7.179260 3.898665

14 H 2.423813 3.044227 4.483702 3.211036 5.803541

15 H 4.135321 5.668750 6.373521 6.718937 8.128049

16 H 3.011364 2.710377 3.180906 3.235932 4.641072

17 H 3.816524 4.183309 4.776802 4.677986 6.363651

18 H 3.033404 3.497325 3.622338 4.595867 5.402319

19 H 4.287729 2.900181 2.403572 3.379536 1.091807

20 H 4.756227 3.049635 2.417795 3.052748 1.089938

21 H 5.866720 4.531261 2.918790 5.232445 2.159138

22 H 5.535080 4.457770 2.952357 5.431017 2.157132

23 H 6.821379 5.421584 4.472980 5.704510 2.747765

24 H 7.096729 5.487925 4.453018 5.525954 2.755572

25 H 8.957423 7.538645 6.259046 7.848652 4.705609

26 H 8.329174 6.959667 5.438161 7.457961 4.229937

27 H 8.096572 6.909357 5.456775 7.594203 4.226791

11 12 13 14 15

11 C 0.000000

12 C 1.531384 0.000000

13 C 2.546011 1.526963 0.000000

14 H 7.133428 8.324262 9.650967 0.000000

15 H 9.058046 10.505655 11.537841 3.949157 0.000000

16 H 5.687433 6.976688 8.133227 2.467677 4.792425

17 H 7.363036 8.703272 9.808671 2.528935 3.801711

18 H 6.216789 7.671393 8.662021 3.076761 3.544321

19 H 2.171110 2.816064 4.228491 5.915487 8.272103

20 H 2.169319 2.771247 4.202757 5.777308 8.518880

21 H 1.096402 2.156938 2.774128 7.244041 9.053919

22 H 1.095667 2.159387 2.769984 7.386579 8.883507

23 H 2.157270 1.096236 2.158067 8.432444 10.672849

24 H 2.157212 1.096096 2.157451 8.313796 10.815729

25 H 3.500097 2.179550 1.093940 10.495243 12.541839

26 H 2.814228 2.178099 1.094734 9.780311 11.582524

27 H 2.816015 2.179095 1.094649 9.884335 11.450596

16 17 18 19 20

16 H 0.000000

17 H 1.766919 0.000000

18 H 1.769522 1.772179 0.000000

19 H 5.191406 6.863599 5.916551 0.000000

20 H 4.558957 6.324760 5.634799 1.766114 0.000000

21 H 5.475280 7.099734 5.967824 3.072345 2.533675

22 H 6.051333 7.629876 6.293329 2.498875 3.069711

23 H 7.380323 9.108858 8.083602 2.585804 3.069419

24 H 6.919861 8.672742 7.833619 3.150768 2.544966

25 H 9.042312 10.748209 9.667527 4.917389 4.876814

26 H 8.034368 9.660994 8.533663 4.791675 4.441980

27 H 8.438950 10.059079 8.767368 4.440159 4.765753

21 22 23 24 25

21 H 0.000000

22 H 1.756726 0.000000

23 H 3.060182 2.512641 0.000000

24 H 2.502795 3.061576 1.753501 0.000000

25 H 3.778466 3.777322 2.502346 2.500820 0.000000

26 H 2.595263 3.129739 3.076985 2.523717 1.765151

27 H 3.141033 2.593150 2.525303 3.077143 1.765370

26 27

26 H 0.000000

27 H 1.765140 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.55D-01

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.114900 -0.434209 -0.145215

2 6 0 -2.844000 0.117002 0.432464

3 8 0 -4.910734 0.203575 -0.796315

4 8 0 -4.276435 -1.754285 0.090420

5 6 0 -2.330238 -0.571950 1.682343

6 16 0 -1.571897 0.036118 -0.980990

7 6 0 -0.118840 0.677361 -0.229962

8 16 0 1.090691 -0.590284 0.141750

9 16 0 -0.003558 2.297047 0.342219

10 6 0 2.688182 0.287603 -0.101808

11 6 0 3.853320 -0.691190 -0.012454

12 6 0 5.204184 0.014897 -0.159921

13 6 0 6.385090 -0.950208 -0.084746

14 1 0 -3.002429 1.180035 0.606430

15 1 0 -5.099338 -2.027329 -0.348361

16 1 0 -1.421086 -0.076094 2.024501

17 1 0 -3.070410 -0.510282 2.486251

18 1 0 -2.103701 -1.622865 1.502254

19 1 0 2.651881 0.766936 -1.082095

20 1 0 2.773607 1.068419 0.653833

21 1 0 3.824584 -1.218076 0.948620

22 1 0 3.754769 -1.456344 -0.790472

23 1 0 5.228581 0.552634 -1.114896

24 1 0 5.301530 0.776027 0.622786

25 1 0 7.338700 -0.424789 -0.190896

26 1 0 6.405545 -1.479532 0.873293

27 1 0 6.334554 -1.704994 -0.875949

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3251836 0.1924522 0.1803106

Leave Link 202 at Sat Aug 17 17:41:08 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.0977411877 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0549849715 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.0427562162 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2323

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.11D-09

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 107

GePol: Fraction of low-weight points (<1% of avg) = 4.61%

GePol: Cavity surface area = 309.318 Ang\*\*2

GePol: Cavity volume = 320.151 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057834867 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.0369727295 Hartrees.

Leave Link 301 at Sat Aug 17 17:41:08 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:41:08 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:41:08 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Lowest energy guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000713 -0.000420 -0.000285 Ang= 0.10 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999869 0.006207 0.010284 0.010851 Ang= 1.85 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 3.76D-02

Max alpha theta= 17.833 degrees.

Max beta theta= 17.881 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 17:41:08 2019, MaxMem= 1342177280 cpu: 4.2

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16188987.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.11D-15 for 2318.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.62D-15 for 686 472.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.88D-15 for 2318.

Iteration 1 A^-1\*A deviation from orthogonality is 3.70D-10 for 796 765.

Iteration 2 A\*A^-1 deviation from unit magnitude is 3.33D-15 for 71.

Iteration 2 A\*A^-1 deviation from orthogonality is 2.72D-15 for 950 873.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.78D-15 for 2116.

Iteration 2 A^-1\*A deviation from orthogonality is 4.45D-16 for 2295 181.

E= -1658.67685311038

DIIS: error= 7.61D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67685311038 IErMin= 1 ErrMin= 7.61D-04

ErrMax= 7.61D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.43D-04 BMatP= 4.43D-04

IDIUse=3 WtCom= 9.92D-01 WtEn= 7.61D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 88.716 Goal= None Shift= 0.000

Gap= 88.735 Goal= None Shift= 0.000

RMSDP=4.67D-05 MaxDP=2.42D-03 OVMax= 3.12D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.65D-05 CP: 1.00D+00

E= -1658.67688758354 Delta-E= -0.000034473154 Rises=F Damp=F

DIIS: error= 8.22D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67688758354 IErMin= 1 ErrMin= 7.61D-04

ErrMax= 8.22D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.48D-04 BMatP= 4.43D-04

IDIUse=3 WtCom= 9.92D-01 WtEn= 8.22D-03

Coeff-Com: 0.502D+00 0.498D+00

Coeff-En: 0.365D+00 0.635D+00

Coeff: 0.501D+00 0.499D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=2.88D-05 MaxDP=2.05D-03 DE=-3.45D-05 OVMax= 2.69D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.18D-05 CP: 1.00D+00 5.99D-01

E= -1658.67695937306 Delta-E= -0.000071789524 Rises=F Damp=F

DIIS: error= 2.34D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67695937306 IErMin= 3 ErrMin= 2.34D-04

ErrMax= 2.34D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.07D-05 BMatP= 4.43D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.34D-03

Coeff-Com: 0.147D-01 0.265D+00 0.720D+00

Coeff-En: 0.000D+00 0.115D+00 0.885D+00

Coeff: 0.147D-01 0.265D+00 0.721D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.02D-05 MaxDP=5.37D-04 DE=-7.18D-05 OVMax= 7.34D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 6.49D-06 CP: 1.00D+00 7.13D-01 7.36D-01

E= -1658.67696827327 Delta-E= -0.000008900210 Rises=F Damp=F

DIIS: error= 1.50D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67696827327 IErMin= 4 ErrMin= 1.50D-04

ErrMax= 1.50D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.05D-05 BMatP= 6.07D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.50D-03

Coeff-Com: -0.134D-01 0.147D+00 0.460D+00 0.406D+00

Coeff-En: 0.000D+00 0.000D+00 0.749D-01 0.925D+00

Coeff: -0.134D-01 0.147D+00 0.459D+00 0.407D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.05D-06 MaxDP=1.88D-04 DE=-8.90D-06 OVMax= 4.21D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.47D-06 CP: 1.00D+00 7.17D-01 7.92D-01 4.50D-01

E= -1658.67697014685 Delta-E= -0.000001873581 Rises=F Damp=F

DIIS: error= 2.90D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67697014685 IErMin= 5 ErrMin= 2.90D-05

ErrMax= 2.90D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.95D-07 BMatP= 1.05D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.944D-02 0.623D-01 0.202D+00 0.233D+00 0.512D+00

Coeff: -0.944D-02 0.623D-01 0.202D+00 0.233D+00 0.512D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=8.53D-07 MaxDP=4.94D-05 DE=-1.87D-06 OVMax= 8.26D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 6.75D-07 CP: 1.00D+00 7.19D-01 7.89D-01 4.79D-01 6.80D-01

E= -1658.67697022879 Delta-E= -0.000000081940 Rises=F Damp=F

DIIS: error= 4.58D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67697022879 IErMin= 6 ErrMin= 4.58D-06

ErrMax= 4.58D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.39D-08 BMatP= 4.95D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.204D-02 0.971D-02 0.324D-01 0.512D-01 0.223D+00 0.685D+00

Coeff: -0.204D-02 0.971D-02 0.324D-01 0.512D-01 0.223D+00 0.685D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.64D-07 MaxDP=1.26D-05 DE=-8.19D-08 OVMax= 2.33D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.86D-07 CP: 1.00D+00 7.20D-01 7.89D-01 4.91D-01 7.56D-01

CP: 8.29D-01

E= -1658.67697023361 Delta-E= -0.000000004817 Rises=F Damp=F

DIIS: error= 1.06D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67697023361 IErMin= 7 ErrMin= 1.06D-06

ErrMax= 1.06D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.91D-09 BMatP= 2.39D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.305D-03 0.326D-03 0.126D-02 0.722D-02 0.609D-01 0.300D+00

Coeff-Com: 0.631D+00

Coeff: -0.305D-03 0.326D-03 0.126D-02 0.722D-02 0.609D-01 0.300D+00

Coeff: 0.631D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.17D-07 MaxDP=3.95D-06 DE=-4.82D-09 OVMax= 9.72D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 8.57D-08 CP: 1.00D+00 7.20D-01 7.90D-01 4.91D-01 7.75D-01

CP: 8.94D-01 7.53D-01

E= -1658.67697023402 Delta-E= -0.000000000417 Rises=F Damp=F

DIIS: error= 3.76D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67697023402 IErMin= 8 ErrMin= 3.76D-07

ErrMax= 3.76D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.06D-10 BMatP= 1.91D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.127D-03-0.127D-02-0.428D-02-0.336D-02 0.211D-03 0.687D-01

Coeff-Com: 0.345D+00 0.594D+00

Coeff: 0.127D-03-0.127D-02-0.428D-02-0.336D-02 0.211D-03 0.687D-01

Coeff: 0.345D+00 0.594D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.26D-08 MaxDP=2.36D-06 DE=-4.17D-10 OVMax= 6.34D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.86D-08 CP: 1.00D+00 7.20D-01 7.90D-01 4.92D-01 7.78D-01

CP: 9.08D-01 8.76D-01 8.19D-01

E= -1658.67697023414 Delta-E= -0.000000000115 Rises=F Damp=F

DIIS: error= 1.48D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67697023414 IErMin= 9 ErrMin= 1.48D-07

ErrMax= 1.48D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.07D-11 BMatP= 4.06D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.976D-04-0.737D-03-0.248D-02-0.247D-02-0.640D-02 0.577D-02

Coeff-Com: 0.117D+00 0.317D+00 0.572D+00

Coeff: 0.976D-04-0.737D-03-0.248D-02-0.247D-02-0.640D-02 0.577D-02

Coeff: 0.117D+00 0.317D+00 0.572D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.25D-08 MaxDP=1.11D-06 DE=-1.15D-10 OVMax= 3.15D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.66D-08 CP: 1.00D+00 7.20D-01 7.90D-01 4.92D-01 7.81D-01

CP: 9.17D-01 9.13D-01 9.45D-01 9.22D-01

E= -1658.67697023414 Delta-E= -0.000000000003 Rises=F Damp=F

DIIS: error= 8.41D-08 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67697023414 IErMin=10 ErrMin= 8.41D-08

ErrMax= 8.41D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.40D-11 BMatP= 5.07D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.171D-04-0.135D-04-0.193D-04-0.288D-03-0.397D-02-0.203D-01

Coeff-Com: -0.498D-01-0.224D-02 0.366D+00 0.710D+00

Coeff: 0.171D-04-0.135D-04-0.193D-04-0.288D-03-0.397D-02-0.203D-01

Coeff: -0.498D-01-0.224D-02 0.366D+00 0.710D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.24D-08 MaxDP=5.73D-07 DE=-3.18D-12 OVMax= 1.38D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 5.66D-09 CP: 1.00D+00 7.20D-01 7.90D-01 4.92D-01 7.82D-01

CP: 9.21D-01 9.35D-01 1.02D+00 1.15D+00 8.15D-01

E= -1658.67697023414 Delta-E= 0.000000000005 Rises=F Damp=F

DIIS: error= 2.04D-08 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=10 EnMin= -1658.67697023414 IErMin=11 ErrMin= 2.04D-08

ErrMax= 2.04D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.46D-12 BMatP= 1.40D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.794D-05 0.117D-03 0.416D-03 0.271D-03-0.550D-03-0.975D-02

Coeff-Com: -0.413D-01-0.511D-01 0.615D-01 0.314D+00 0.727D+00

Coeff: -0.794D-05 0.117D-03 0.416D-03 0.271D-03-0.550D-03-0.975D-02

Coeff: -0.413D-01-0.511D-01 0.615D-01 0.314D+00 0.727D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.77D-09 MaxDP=2.27D-07 DE= 5.46D-12 OVMax= 7.89D-07

Error on total polarization charges = 0.04165

SCF Done: E(UB3LYP) = -1658.67697023 A.U. after 11 cycles

NFock= 11 Conv=0.58D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655250643978D+03 PE=-6.146849173403D+03 EE= 1.730884586461D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.63

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:41:32 2019, MaxMem= 1342177280 cpu: 275.6

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 337

Leave Link 701 at Sat Aug 17 17:41:33 2019, MaxMem= 1342177280 cpu: 10.2

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:41:33 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:41:36 2019, MaxMem= 1342177280 cpu: 36.1

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.37917785D+00-2.91834160D+00 5.98385368D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.001605045 -0.000784704 -0.000068322

2 6 -0.000184787 -0.000023532 0.000719034

3 8 -0.001291369 0.001086992 -0.000565320

4 8 -0.000047251 -0.000350721 0.000300533

5 6 0.000172472 -0.000072254 -0.000012808

6 16 0.000173059 0.000274011 -0.000337367

7 6 -0.000093839 -0.000102526 -0.000275114

8 16 0.000333616 -0.000049411 0.000125230

9 16 0.000005736 0.000061009 0.000180785

10 6 -0.000329931 -0.000085027 -0.000031261

11 6 -0.000001683 -0.000033739 -0.000002685

12 6 -0.000083089 0.000026689 -0.000015083

13 6 0.000094073 -0.000109680 -0.000044508

14 1 -0.000101504 0.000157421 0.000163789

15 1 -0.000296367 -0.000135699 -0.000158228

16 1 0.000155836 0.000018073 0.000060849

17 1 -0.000139665 0.000052080 0.000066500

18 1 -0.000067942 -0.000179840 -0.000061193

19 1 0.000150630 0.000268470 -0.000212648

20 1 -0.000105175 0.000006594 0.000251487

21 1 -0.000045267 -0.000018588 0.000167212

22 1 0.000042097 -0.000117474 -0.000183174

23 1 -0.000013612 0.000080460 -0.000116504

24 1 0.000051167 0.000048200 0.000185997

25 1 0.000134502 0.000096024 -0.000033254

26 1 -0.000022819 -0.000100747 0.000112471

27 1 -0.000093931 -0.000012083 -0.000216418

-------------------------------------------------------------------

Cartesian Forces: Max 0.001605045 RMS 0.000324824

Leave Link 716 at Sat Aug 17 17:41:36 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.001745860 RMS 0.000214151

Search for a local minimum.

Step number 26 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .21415D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 26 19

ITU= 0 -1 0 0 -1 1 -1 1 -1 1 1 -1 1 -1 1 1 -1 0 0 -1

ITU= 0 0 -1 -1 0 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.74214.

Iteration 1 RMS(Cart)= 0.01604301 RMS(Int)= 0.00007428

Iteration 2 RMS(Cart)= 0.00020046 RMS(Int)= 0.00000014

Iteration 3 RMS(Cart)= 0.00000003 RMS(Int)= 0.00000014

ITry= 1 IFail=0 DXMaxC= 5.41D-02 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=T

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83631 0.00031 0.00099 0.00000 0.00099 2.83730

R2 2.28653 0.00175 0.00125 0.00000 0.00125 2.28778

R3 2.55233 0.00058 0.00069 0.00000 0.00069 2.55302

R4 2.86641 0.00011 0.00018 0.00000 0.00018 2.86660

R5 3.59676 0.00048 0.00012 0.00000 0.00012 3.59688

R6 2.05746 0.00021 0.00050 0.00000 0.00050 2.05796

R7 1.83630 0.00034 0.00055 0.00000 0.00055 1.83684

R8 2.06102 0.00018 0.00034 0.00000 0.00034 2.06136

R9 2.06830 0.00015 0.00038 0.00000 0.00038 2.06868

R10 2.05987 0.00013 0.00037 0.00000 0.00037 2.06024

R11 3.32001 -0.00006 0.00027 0.00000 0.00027 3.32028

R12 3.38470 0.00014 -0.00058 0.00000 -0.00058 3.38412

R13 3.25344 0.00011 0.00055 0.00000 0.00055 3.25399

R14 3.47524 -0.00019 0.00091 0.00000 0.00091 3.47615

R15 2.88056 0.00017 0.00035 0.00000 0.00035 2.88090

R16 2.06322 0.00033 0.00044 0.00000 0.00044 2.06365

R17 2.05968 0.00018 0.00049 0.00000 0.00049 2.06017

R18 2.89390 0.00006 0.00032 0.00000 0.00032 2.89422

R19 2.07190 0.00016 0.00038 0.00000 0.00038 2.07228

R20 2.07051 0.00020 0.00033 0.00000 0.00033 2.07084

R21 2.88554 0.00018 0.00030 0.00000 0.00030 2.88584

R22 2.07159 0.00014 0.00036 0.00000 0.00036 2.07194

R23 2.07132 0.00018 0.00034 0.00000 0.00034 2.07166

R24 2.06725 0.00016 0.00037 0.00000 0.00037 2.06761

R25 2.06875 0.00018 0.00038 0.00000 0.00038 2.06913

R26 2.06859 0.00016 0.00037 0.00000 0.00037 2.06895

A1 2.17786 -0.00006 -0.00052 0.00000 -0.00052 2.17734

A2 1.97476 0.00014 0.00097 0.00000 0.00097 1.97573

A3 2.12986 -0.00007 -0.00032 0.00000 -0.00032 2.12954

A4 2.02321 0.00006 0.00009 0.00000 0.00009 2.02331

A5 1.83848 -0.00020 -0.00068 0.00000 -0.00068 1.83780

A6 1.87220 0.00006 -0.00064 0.00000 -0.00064 1.87155

A7 1.94577 0.00016 0.00055 0.00000 0.00055 1.94631

A8 1.94024 -0.00010 -0.00016 0.00000 -0.00016 1.94008

A9 1.83113 0.00001 0.00087 0.00000 0.00087 1.83200

A10 1.87249 0.00017 0.00065 0.00000 0.00065 1.87314

A11 1.91171 0.00003 -0.00012 0.00000 -0.00012 1.91159

A12 1.92899 -0.00018 -0.00031 0.00000 -0.00031 1.92867

A13 1.95213 0.00002 0.00017 0.00000 0.00017 1.95230

A14 1.88356 0.00004 0.00017 0.00000 0.00017 1.88373

A15 1.89328 0.00003 0.00002 0.00000 0.00002 1.89330

A16 1.89254 0.00006 0.00008 0.00000 0.00008 1.89261

A17 1.79242 -0.00009 0.00048 0.00000 0.00048 1.79290

A18 1.97025 0.00000 0.00155 0.00000 0.00155 1.97180

A19 2.14222 0.00001 -0.00021 0.00000 -0.00021 2.14200

A20 2.15512 -0.00006 -0.00091 0.00000 -0.00091 2.15421

A21 1.79391 0.00034 -0.00081 0.00000 -0.00081 1.79311

A22 1.92803 -0.00044 0.00050 0.00000 0.00050 1.92853

A23 1.87508 0.00028 -0.00044 0.00000 -0.00044 1.87464

A24 1.89467 0.00003 0.00043 0.00000 0.00043 1.89510

A25 1.93901 0.00002 -0.00035 0.00000 -0.00035 1.93866

A26 1.93848 0.00014 -0.00008 0.00000 -0.00008 1.93840

A27 1.88659 -0.00002 -0.00006 0.00000 -0.00006 1.88653

A28 1.95255 0.00024 -0.00015 0.00000 -0.00015 1.95241

A29 1.91763 -0.00012 0.00032 0.00000 0.00032 1.91796

A30 1.91563 -0.00003 -0.00030 0.00000 -0.00030 1.91533

A31 1.90615 -0.00003 -0.00013 0.00000 -0.00013 1.90602

A32 1.91023 -0.00014 -0.00002 0.00000 -0.00002 1.91021

A33 1.85927 0.00006 0.00030 0.00000 0.00030 1.85956

A34 1.96713 -0.00014 0.00014 0.00000 0.00014 1.96728

A35 1.90677 0.00002 -0.00030 0.00000 -0.00030 1.90647

A36 1.90684 0.00007 -0.00002 0.00000 -0.00002 1.90682

A37 1.91316 0.00002 -0.00030 0.00000 -0.00030 1.91286

A38 1.91246 0.00004 0.00024 0.00000 0.00024 1.91269

A39 1.85404 0.00000 0.00025 0.00000 0.00025 1.85428

A40 1.94530 0.00002 -0.00004 0.00000 -0.00004 1.94526

A41 1.94243 -0.00002 -0.00009 0.00000 -0.00009 1.94234

A42 1.94391 -0.00015 -0.00021 0.00000 -0.00021 1.94370

A43 1.87639 0.00002 0.00005 0.00000 0.00005 1.87644

A44 1.87684 0.00006 0.00014 0.00000 0.00014 1.87697

A45 1.87549 0.00008 0.00019 0.00000 0.00019 1.87568

D1 2.66453 -0.00018 0.00202 0.00000 0.00202 2.66655

D2 -1.45882 -0.00009 0.00227 0.00000 0.00227 -1.45655

D3 0.48536 -0.00014 0.00268 0.00000 0.00268 0.48805

D4 -0.51680 0.00014 0.00590 0.00000 0.00590 -0.51091

D5 1.64303 0.00023 0.00615 0.00000 0.00615 1.64917

D6 -2.69597 0.00018 0.00656 0.00000 0.00656 -2.68941

D7 -3.10116 -0.00018 -0.00201 0.00000 -0.00201 -3.10317

D8 0.00193 0.00013 0.00174 0.00000 0.00174 0.00367

D9 -3.11841 -0.00005 -0.00076 0.00000 -0.00076 -3.11917

D10 -1.04536 -0.00009 -0.00082 0.00000 -0.00082 -1.04618

D11 1.06513 -0.00012 -0.00082 0.00000 -0.00082 1.06431

D12 1.06187 0.00005 -0.00035 0.00000 -0.00035 1.06152

D13 3.13492 0.00001 -0.00041 0.00000 -0.00041 3.13451

D14 -1.03778 -0.00002 -0.00041 0.00000 -0.00041 -1.03819

D15 -0.97463 -0.00001 -0.00169 0.00000 -0.00169 -0.97631

D16 1.09842 -0.00004 -0.00174 0.00000 -0.00174 1.09668

D17 -3.07427 -0.00008 -0.00175 0.00000 -0.00175 -3.07602

D18 -3.13209 0.00011 -0.01480 0.00000 -0.01480 3.13629

D19 -0.92392 0.00015 -0.01481 0.00000 -0.01481 -0.93874

D20 1.17792 0.00012 -0.01417 0.00000 -0.01417 1.16375

D21 1.84321 -0.00028 0.00327 0.00000 0.00327 1.84647

D22 -1.11538 0.00007 0.00090 0.00000 0.00090 -1.11448

D23 2.55856 0.00026 -0.00819 0.00000 -0.00819 2.55037

D24 -0.76761 -0.00008 -0.00572 0.00000 -0.00572 -0.77332

D25 -3.00730 -0.00003 0.01374 0.00000 0.01374 -2.99355

D26 -0.88974 -0.00009 0.01334 0.00000 0.01334 -0.87641

D27 1.14647 0.00005 0.01325 0.00000 0.01325 1.15972

D28 -3.10520 0.00003 0.00195 0.00000 0.00195 -3.10325

D29 -0.98498 0.00007 0.00191 0.00000 0.00191 -0.98307

D30 1.05398 0.00006 0.00228 0.00000 0.00228 1.05626

D31 1.09880 -0.00005 0.00240 0.00000 0.00240 1.10120

D32 -3.06417 -0.00001 0.00236 0.00000 0.00236 -3.06181

D33 -1.02521 -0.00002 0.00273 0.00000 0.00273 -1.02248

D34 -1.00177 -0.00014 0.00277 0.00000 0.00277 -0.99901

D35 1.11844 -0.00009 0.00273 0.00000 0.00273 1.12117

D36 -3.12578 -0.00010 0.00310 0.00000 0.00310 -3.12268

D37 -3.13336 0.00004 0.00546 0.00000 0.00546 -3.12790

D38 -1.00205 -0.00002 0.00496 0.00000 0.00496 -0.99709

D39 1.01937 0.00003 0.00508 0.00000 0.00508 1.02445

D40 1.02301 0.00005 0.00524 0.00000 0.00524 1.02825

D41 -3.12888 -0.00001 0.00474 0.00000 0.00474 -3.12414

D42 -1.10745 0.00004 0.00485 0.00000 0.00485 -1.10259

D43 -1.00625 0.00007 0.00497 0.00000 0.00497 -1.00128

D44 1.12506 0.00001 0.00447 0.00000 0.00447 1.12952

D45 -3.13670 0.00006 0.00458 0.00000 0.00458 -3.13212

D46 -3.14020 -0.00004 0.00113 0.00000 0.00113 -3.13907

D47 -1.04564 -0.00002 0.00110 0.00000 0.00110 -1.04454

D48 1.04685 -0.00002 0.00114 0.00000 0.00114 1.04798

D49 1.01528 0.00001 0.00164 0.00000 0.00164 1.01692

D50 3.10985 0.00004 0.00160 0.00000 0.00160 3.11145

D51 -1.08085 0.00003 0.00164 0.00000 0.00164 -1.07921

D52 -1.01292 -0.00002 0.00138 0.00000 0.00138 -1.01154

D53 1.08164 0.00000 0.00135 0.00000 0.00135 1.08299

D54 -3.10906 0.00000 0.00138 0.00000 0.00138 -3.10768

Item Value Threshold Converged?

Maximum Force 0.001746 0.000450 NO

RMS Force 0.000214 0.000300 YES

Maximum Displacement 0.054100 0.001800 NO

RMS Displacement 0.016014 0.001200 NO

Predicted change in Energy=-1.241401D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:41:36 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.106175 -0.413602 -0.203852

2 6 0 -2.839631 0.059604 0.449021

3 8 0 -4.888730 0.300196 -0.790151

4 8 0 -4.282955 -1.750116 -0.116204

5 6 0 -2.346331 -0.770460 1.618956

6 16 0 -1.550170 0.130894 -0.949222

7 6 0 -0.109064 0.696430 -0.118260

8 16 0 1.106215 -0.595035 0.131105

9 16 0 -0.009403 2.248324 0.621175

10 6 0 2.699119 0.313315 -0.014915

11 6 0 3.870049 -0.662667 -0.037530

12 6 0 5.216772 0.063664 -0.104168

13 6 0 6.403309 -0.896751 -0.147025

14 1 0 -2.995384 1.097096 0.741124

15 1 0 -5.102351 -1.965543 -0.592646

16 1 0 -1.438526 -0.323293 2.026175

17 1 0 -3.096798 -0.794442 2.415566

18 1 0 -2.123894 -1.796126 1.323764

19 1 0 2.658093 0.898878 -0.935774

20 1 0 2.782289 1.005675 0.823088

21 1 0 3.845470 -1.295682 0.857582

22 1 0 3.775079 -1.334826 -0.897794

23 1 0 5.234921 0.710368 -0.989376

24 1 0 5.312583 0.727780 0.762777

25 1 0 7.353856 -0.356761 -0.191757

26 1 0 6.429255 -1.536424 0.741249

27 1 0 6.354563 -1.552136 -1.022683

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.501433 0.000000

3 O 1.210639 2.406707 0.000000

4 O 1.351001 2.382803 2.241639 0.000000

5 C 2.558716 1.516937 3.662498 2.778672 0.000000

6 S 2.717575 1.903385 3.346632 3.420560 2.835815

7 C 4.149264 2.860656 4.842896 4.838073 3.189835

8 S 5.226292 4.012396 6.131029 5.517112 3.763582

9 S 4.954802 3.581945 5.440118 5.898686 3.945867

10 C 6.846615 5.563934 7.627360 7.281303 5.413010

11 C 7.981845 6.765960 8.843628 8.225583 6.434202

12 C 9.335687 8.075374 10.131520 9.671337 7.801631

13 C 10.520737 9.311381 11.373497 10.720327 8.926973

14 H 2.099772 1.089024 2.562150 3.240287 2.163244

15 H 1.884688 3.210326 2.284342 0.972016 3.730288

16 H 3.478150 2.144090 4.497148 3.836195 1.090824

17 H 2.832884 2.159359 3.832216 2.954681 1.094698

18 H 2.859094 2.172829 4.062945 2.595606 1.090232

19 H 6.929187 5.731231 7.571933 7.474424 5.861535

20 H 7.107734 5.713226 7.870500 7.641618 5.485509

21 H 8.070524 6.833322 9.030398 8.199150 6.260507

22 H 7.965197 6.892948 8.817396 8.106495 6.642605

23 H 9.441209 8.227446 10.133915 9.869466 8.153013

24 H 9.536778 8.185567 10.327691 9.949217 7.850907

25 H 11.460178 10.222090 12.274794 11.720175 9.876409

26 H 10.637163 9.409833 11.567850 10.748597 8.852569

27 H 10.554325 9.449699 11.397229 10.677906 9.126600

6 7 8 9 10

6 S 0.000000

7 C 1.757018 0.000000

8 S 2.958118 1.790801 0.000000

9 S 3.053461 1.721939 3.093455 0.000000

10 C 4.354615 2.836080 1.839501 3.388947 0.000000

11 C 5.553350 4.205592 2.769800 4.894682 1.524509

12 C 6.819834 5.363313 4.169642 5.710671 2.531574

13 C 8.059615 6.704480 5.312964 7.183627 3.899068

14 H 2.424759 3.038078 4.478677 3.202468 5.797696

15 H 4.140070 5.678385 6.399094 6.720726 8.148000

16 H 3.011932 2.721379 3.184469 3.260312 4.657405

17 H 3.817080 4.191602 4.787886 4.691511 6.381773

18 H 3.034638 3.514514 3.646733 4.617606 5.431691

19 H 4.277787 2.892486 2.403816 3.370553 1.092039

20 H 4.761987 3.056418 2.418747 3.062431 1.090197

21 H 5.866224 4.534216 2.919279 5.241747 2.159686

22 H 5.523518 4.451992 2.954447 5.428492 2.157205

23 H 6.809909 5.414537 4.472780 5.697553 2.745453

24 H 7.098211 5.492856 4.454479 5.536753 2.758039

25 H 8.949482 7.537227 6.260513 7.852700 4.706043

26 H 8.325195 6.962328 5.439967 7.469608 4.231694

27 H 8.082251 6.903079 5.458243 7.592484 4.225845

11 12 13 14 15

11 C 0.000000

12 C 1.531555 0.000000

13 C 2.546407 1.527123 0.000000

14 H 7.130024 8.319976 9.648817 0.000000

15 H 9.083479 10.528085 11.563784 3.949431 0.000000

16 H 5.705701 6.998649 8.157575 2.468333 4.793623

17 H 7.387287 8.729310 9.840192 2.528232 3.800403

18 H 6.250217 7.706049 8.699730 3.077287 3.545777

19 H 2.171198 2.817088 4.227653 5.900261 8.279320

20 H 2.169620 2.770180 4.203824 5.778977 8.544002

21 H 1.096604 2.157141 2.776855 7.248188 9.089299

22 H 1.095842 2.159652 2.768241 7.378310 8.905036

23 H 2.157339 1.096425 2.158128 8.419151 10.685367

24 H 2.157485 1.096277 2.157898 8.316200 10.842602

25 H 3.500610 2.179806 1.094134 10.492413 12.566064

26 H 2.814158 2.178331 1.094937 9.785666 11.616426

27 H 2.816822 2.179231 1.094843 9.876788 11.472432

16 17 18 19 20

16 H 0.000000

17 H 1.767335 0.000000

18 H 1.769844 1.772553 0.000000

19 H 5.200878 6.871505 5.935989 0.000000

20 H 4.585722 6.351383 5.671984 1.766472 0.000000

21 H 5.498341 7.132576 6.008417 3.072797 2.535309

22 H 6.062546 7.648076 6.320285 2.497705 3.070018

23 H 7.395734 9.125548 8.110813 2.584269 3.063925

24 H 6.948266 8.704399 7.873119 3.156052 2.546224

25 H 9.067873 10.779882 9.705479 4.917354 4.877025

26 H 8.063789 9.700493 8.576896 4.792156 4.446272

27 H 8.458003 10.085826 8.800544 4.436092 4.765544

21 22 23 24 25

21 H 0.000000

22 H 1.757223 0.000000

23 H 3.060403 2.514427 0.000000

24 H 2.501162 3.061986 1.753959 0.000000

25 H 3.780405 3.776605 2.502967 2.500831 0.000000

26 H 2.597583 3.125981 3.077267 2.524686 1.765500

27 H 3.145904 2.591632 2.524606 3.077597 1.765770

26 27

26 H 0.000000

27 H 1.765583 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 7.36D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.117751 -0.424398 -0.157932

2 6 0 -2.845385 0.113492 0.430335

3 8 0 -4.901185 0.222486 -0.816278

4 8 0 -4.299098 -1.741781 0.080436

5 6 0 -2.348027 -0.582015 1.683333

6 16 0 -1.564347 0.021356 -0.974417

7 6 0 -0.115967 0.670223 -0.220573

8 16 0 1.095882 -0.590482 0.165450

9 16 0 -0.005788 2.294935 0.339110

10 6 0 2.691316 0.288521 -0.090889

11 6 0 3.858339 -0.689076 -0.010334

12 6 0 5.207393 0.019095 -0.165921

13 6 0 6.389957 -0.945380 -0.107319

14 1 0 -2.995353 1.177933 0.604826

15 1 0 -5.122248 -2.005709 -0.364065

16 1 0 -1.436011 -0.095997 2.032491

17 1 0 -3.093631 -0.512924 2.481873

18 1 0 -2.131350 -1.635352 1.504062

19 1 0 2.646827 0.767042 -1.071494

20 1 0 2.782324 1.070309 0.663468

21 1 0 3.836883 -1.217346 0.950400

22 1 0 3.755469 -1.453240 -0.789013

23 1 0 5.222533 0.562109 -1.118315

24 1 0 5.311115 0.776014 0.620297

25 1 0 7.342269 -0.418123 -0.217921

26 1 0 6.418958 -1.481262 0.847079

27 1 0 6.333279 -1.694815 -0.903445

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3281813 0.1920412 0.1800483

Leave Link 202 at Sat Aug 17 17:41:36 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1101.5995917326 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0549324405 Hartrees.

Nuclear repulsion after empirical dispersion term = 1101.5446592920 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2318

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.15D-08

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 103

GePol: Fraction of low-weight points (<1% of avg) = 4.44%

GePol: Cavity surface area = 309.427 Ang\*\*2

GePol: Cavity volume = 320.164 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057979033 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1101.5388613887 Hartrees.

Leave Link 301 at Sat Aug 17 17:41:37 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:41:37 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:41:37 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Lowest energy guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000191 -0.000108 -0.000073 Ang= 0.03 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000522 0.000312 0.000212 Ang= -0.07 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 2.58D-01

Max alpha theta= 0.630 degrees.

Max beta theta= 0.628 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 17:41:37 2019, MaxMem= 1342177280 cpu: 4.3

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16119372.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.44D-15 for 2290.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.61D-15 for 962 22.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.77D-15 for 2287.

Iteration 1 A^-1\*A deviation from orthogonality is 1.52D-12 for 918 911.

E= -1658.67697579767

DIIS: error= 4.97D-06 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67697579767 IErMin= 1 ErrMin= 4.97D-06

ErrMax= 4.97D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.12D-08 BMatP= 2.12D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 88.693 Goal= None Shift= 0.000

Gap= 88.720 Goal= None Shift= 0.000

RMSDP=3.19D-07 MaxDP=1.57D-05 OVMax= 2.02D-05

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.18D-07 CP: 1.00D+00

E= -1658.67697579998 Delta-E= -0.000000002306 Rises=F Damp=F

DIIS: error= 5.20D-06 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67697579998 IErMin= 1 ErrMin= 4.97D-06

ErrMax= 5.20D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.90D-08 BMatP= 2.12D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.482D+00 0.518D+00

Coeff: 0.482D+00 0.518D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.02D-07 MaxDP=1.38D-05 DE=-2.31D-09 OVMax= 1.81D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.61D-07 CP: 1.00D+00 6.19D-01

E= -1658.67697580286 Delta-E= -0.000000002884 Rises=F Damp=F

DIIS: error= 1.69D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67697580286 IErMin= 3 ErrMin= 1.69D-06

ErrMax= 1.69D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.68D-09 BMatP= 1.90D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.182D-01 0.302D+00 0.680D+00

Coeff: 0.182D-01 0.302D+00 0.680D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=7.98D-08 MaxDP=3.97D-06 DE=-2.88D-09 OVMax= 6.03D-06

Cycle 4 Pass 1 IDiag 1:

RMSU= 4.85D-08 CP: 1.00D+00 7.42D-01 6.94D-01

E= -1658.67697580339 Delta-E= -0.000000000532 Rises=F Damp=F

DIIS: error= 1.15D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67697580339 IErMin= 4 ErrMin= 1.15D-06

ErrMax= 1.15D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.82D-10 BMatP= 3.68D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.141D-01 0.168D+00 0.437D+00 0.409D+00

Coeff: -0.141D-01 0.168D+00 0.437D+00 0.409D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.00D-08 MaxDP=1.30D-06 DE=-5.32D-10 OVMax= 3.02D-06

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.10D-08 CP: 1.00D+00 7.48D-01 7.53D-01 4.61D-01

E= -1658.67697580352 Delta-E= -0.000000000125 Rises=F Damp=F

DIIS: error= 1.95D-07 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67697580352 IErMin= 5 ErrMin= 1.95D-07

ErrMax= 1.95D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.31D-11 BMatP= 5.82D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.933D-02 0.671D-01 0.183D+00 0.223D+00 0.536D+00

Coeff: -0.933D-02 0.671D-01 0.183D+00 0.223D+00 0.536D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.90D-09 MaxDP=3.67D-07 DE=-1.25D-10 OVMax= 5.60D-07

Error on total polarization charges = 0.04168

SCF Done: E(UB3LYP) = -1658.67697580 A.U. after 5 cycles

NFock= 5 Conv=0.59D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655239419989D+03 PE=-6.145844079511D+03 EE= 1.730388822330D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.64

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:41:50 2019, MaxMem= 1342177280 cpu: 138.5

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 338

Leave Link 701 at Sat Aug 17 17:41:50 2019, MaxMem= 1342177280 cpu: 10.2

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:41:51 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:41:54 2019, MaxMem= 1342177280 cpu: 36.1

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.36357764D+00-2.91274849D+00 5.90343411D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000611818 -0.000315733 -0.000075908

2 6 -0.000310229 -0.000185310 0.000428847

3 8 -0.000467049 0.000385522 -0.000196628

4 8 0.000051182 -0.000104571 0.000124276

5 6 0.000148720 -0.000027712 -0.000035192

6 16 0.000140084 0.000286473 -0.000189519

7 6 -0.000122922 0.000041932 -0.000179905

8 16 0.000360537 -0.000041491 0.000030540

9 16 -0.000047664 -0.000054993 0.000218435

10 6 -0.000245761 -0.000016486 -0.000025400

11 6 -0.000024804 -0.000070183 0.000016163

12 6 -0.000071022 0.000056625 -0.000058132

13 6 0.000049831 -0.000104846 -0.000005566

14 1 0.000019085 0.000063323 -0.000010934

15 1 -0.000087793 0.000034377 -0.000039663

16 1 0.000093973 -0.000025508 0.000058313

17 1 -0.000026129 0.000021972 0.000012242

18 1 -0.000061853 -0.000054732 -0.000037759

19 1 0.000117188 0.000157064 -0.000070257

20 1 -0.000116868 -0.000073262 0.000109199

21 1 -0.000048023 0.000029820 0.000055037

22 1 0.000035462 -0.000051501 -0.000067639

23 1 -0.000003469 0.000026500 -0.000017592

24 1 0.000040113 -0.000010316 0.000068872

25 1 0.000025600 0.000030192 -0.000028125

26 1 -0.000001573 -0.000030333 0.000004445

27 1 -0.000058434 0.000033176 -0.000088149

-------------------------------------------------------------------

Cartesian Forces: Max 0.000611818 RMS 0.000151821

Leave Link 716 at Sat Aug 17 17:41:54 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000617165 RMS 0.000134740

Search for a local minimum.

Step number 27 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .13474D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 27

ITU= 0 0 -1 0 0 -1 1 -1 1 -1 1 1 -1 1 -1 1 1 -1 0 0

ITU= -1 0 0 -1 -1 0 0

Eigenvalues --- 0.00000 0.00100 0.00190 0.00228 0.00397

Eigenvalues --- 0.00457 0.00680 0.00799 0.01199 0.01832

Eigenvalues --- 0.02315 0.03528 0.03652 0.03956 0.04414

Eigenvalues --- 0.04739 0.04825 0.05036 0.05423 0.05471

Eigenvalues --- 0.05481 0.05534 0.05805 0.06176 0.08037

Eigenvalues --- 0.08238 0.08375 0.11308 0.11770 0.12233

Eigenvalues --- 0.13231 0.14488 0.14999 0.15952 0.16002

Eigenvalues --- 0.16079 0.16097 0.16220 0.16330 0.17681

Eigenvalues --- 0.19046 0.19710 0.21868 0.22014 0.22438

Eigenvalues --- 0.23706 0.24235 0.25386 0.25581 0.26540

Eigenvalues --- 0.26898 0.27722 0.29038 0.29376 0.29587

Eigenvalues --- 0.29962 0.30500 0.32018 0.33707 0.33859

Eigenvalues --- 0.33878 0.33912 0.33948 0.34036 0.34047

Eigenvalues --- 0.34115 0.34140 0.34325 0.34457 0.34560

Eigenvalues --- 0.34670 0.38828 0.52769 0.55775 1.20859

Eigenvalue 1 is 4.30D-07 Eigenvector:

D1 D2 D3 D4 D5

1 0.33781 0.32646 0.31076 0.28408 0.27273

D26 D25 D6 D27 D19

1 0.26927 0.26105 0.25703 0.25299 0.17514

En-DIIS/RFO-DIIS IScMMF= 0 using points: 27 26

RFO step: Lambda=-8.03017536D-06.

NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=F DC= 5.57D-06 SmlDif= 1.00D-05

RMS Error= 0.9588567433D-03 NUsed= 2 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: -0.03739 1.03739

Iteration 1 RMS(Cart)= 0.15469667 RMS(Int)= 0.01319955

Iteration 2 RMS(Cart)= 0.04024012 RMS(Int)= 0.00042289

Iteration 3 RMS(Cart)= 0.00076362 RMS(Int)= 0.00008880

Iteration 4 RMS(Cart)= 0.00000024 RMS(Int)= 0.00008880

ITry= 1 IFail=0 DXMaxC= 6.21D-01 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83730 0.00000 -0.00102 0.00903 0.00801 2.84531

R2 2.28778 0.00062 -0.00129 0.00248 0.00118 2.28896

R3 2.55302 0.00013 -0.00071 0.00596 0.00524 2.55827

R4 2.86660 0.00004 -0.00019 0.00243 0.00224 2.86883

R5 3.59688 0.00020 -0.00012 0.00373 0.00360 3.60048

R6 2.05796 0.00005 -0.00051 -0.00019 -0.00071 2.05725

R7 1.83684 0.00007 -0.00057 0.00164 0.00107 1.83792

R8 2.06136 0.00010 -0.00035 -0.00048 -0.00083 2.06053

R9 2.06868 0.00003 -0.00039 0.00233 0.00194 2.07062

R10 2.06024 0.00001 -0.00039 0.00170 0.00131 2.06155

R11 3.32028 -0.00015 -0.00028 0.01114 0.01086 3.33114

R12 3.38412 0.00014 0.00060 -0.00039 0.00021 3.38433

R13 3.25399 0.00002 -0.00058 0.00311 0.00254 3.25653

R14 3.47615 -0.00029 -0.00095 -0.00437 -0.00532 3.47083

R15 2.88090 0.00005 -0.00036 0.00348 0.00312 2.88403

R16 2.06365 0.00015 -0.00045 0.00386 0.00341 2.06706

R17 2.06017 0.00002 -0.00051 0.00177 0.00126 2.06143

R18 2.89422 -0.00002 -0.00033 0.00038 0.00005 2.89427

R19 2.07228 0.00004 -0.00039 0.00206 0.00167 2.07395

R20 2.07084 0.00007 -0.00034 0.00228 0.00193 2.07278

R21 2.88584 0.00007 -0.00031 0.00368 0.00337 2.88921

R22 2.07194 0.00003 -0.00037 0.00118 0.00080 2.07275

R23 2.07166 0.00005 -0.00036 0.00189 0.00154 2.07320

R24 2.06761 0.00004 -0.00038 0.00182 0.00144 2.06905

R25 2.06913 0.00005 -0.00040 0.00174 0.00135 2.07048

R26 2.06895 0.00003 -0.00038 0.00161 0.00123 2.07018

A1 2.17734 0.00009 0.00054 0.00157 0.00184 2.17918

A2 1.97573 -0.00010 -0.00101 -0.00344 -0.00473 1.97100

A3 2.12954 0.00001 0.00034 0.00338 0.00344 2.13298

A4 2.02331 0.00001 -0.00010 -0.02032 -0.02048 2.00282

A5 1.83780 -0.00002 0.00071 0.00786 0.00864 1.84644

A6 1.87155 0.00008 0.00067 -0.00377 -0.00324 1.86831

A7 1.94631 0.00002 -0.00057 0.01013 0.00960 1.95592

A8 1.94008 -0.00004 0.00016 -0.00052 -0.00053 1.93955

A9 1.83200 -0.00006 -0.00090 0.00939 0.00846 1.84047

A10 1.87314 -0.00003 -0.00068 0.01625 0.01558 1.88872

A11 1.91159 0.00006 0.00012 0.00433 0.00444 1.91603

A12 1.92867 -0.00009 0.00033 -0.00878 -0.00845 1.92022

A13 1.95230 0.00000 -0.00018 0.00298 0.00278 1.95508

A14 1.88373 0.00000 -0.00018 -0.00152 -0.00169 1.88203

A15 1.89330 0.00001 -0.00002 0.00490 0.00484 1.89814

A16 1.89261 0.00004 -0.00008 -0.00188 -0.00196 1.89065

A17 1.79290 -0.00051 -0.00050 0.01254 0.01204 1.80493

A18 1.97180 -0.00021 -0.00160 -0.00298 -0.00502 1.96678

A19 2.14200 0.00009 0.00022 0.00380 0.00356 2.14557

A20 2.15421 0.00003 0.00095 -0.00938 -0.00886 2.14535

A21 1.79311 0.00044 0.00084 0.01265 0.01349 1.80659

A22 1.92853 -0.00049 -0.00052 -0.02150 -0.02204 1.90649

A23 1.87464 0.00025 0.00046 0.00840 0.00887 1.88351

A24 1.89510 0.00007 -0.00044 0.00275 0.00223 1.89733

A25 1.93866 0.00010 0.00036 0.00468 0.00506 1.94372

A26 1.93840 0.00012 0.00008 0.00161 0.00163 1.94003

A27 1.88653 -0.00004 0.00006 0.00480 0.00483 1.89135

A28 1.95241 0.00021 0.00015 0.01456 0.01471 1.96711

A29 1.91796 -0.00014 -0.00034 -0.00562 -0.00601 1.91195

A30 1.91533 0.00000 0.00031 -0.00399 -0.00366 1.91167

A31 1.90602 0.00000 0.00014 0.00218 0.00232 1.90834

A32 1.91021 -0.00013 0.00002 -0.00719 -0.00715 1.90306

A33 1.85956 0.00005 -0.00031 -0.00071 -0.00104 1.85853

A34 1.96728 -0.00015 -0.00015 -0.00768 -0.00785 1.95943

A35 1.90647 0.00003 0.00031 -0.00194 -0.00168 1.90479

A36 1.90682 0.00008 0.00002 0.00827 0.00830 1.91512

A37 1.91286 0.00004 0.00031 -0.00378 -0.00350 1.90936

A38 1.91269 0.00002 -0.00024 0.00348 0.00326 1.91595

A39 1.85428 -0.00001 -0.00025 0.00226 0.00201 1.85629

A40 1.94526 0.00000 0.00005 0.00316 0.00320 1.94846

A41 1.94234 0.00000 0.00009 0.00056 0.00065 1.94299

A42 1.94370 -0.00008 0.00022 -0.00576 -0.00554 1.93816

A43 1.87644 0.00001 -0.00005 -0.00033 -0.00038 1.87606

A44 1.87697 0.00003 -0.00014 0.00019 0.00006 1.87703

A45 1.87568 0.00004 -0.00019 0.00232 0.00212 1.87780

D1 2.66655 -0.00005 -0.00210 -0.17198 -0.17402 2.49253

D2 -1.45655 -0.00003 -0.00235 -0.16617 -0.16852 -1.62508

D3 0.48805 -0.00007 -0.00278 -0.15369 -0.15652 0.33153

D4 -0.51091 0.00009 -0.00612 -0.12457 -0.13065 -0.64156

D5 1.64917 0.00011 -0.00638 -0.11877 -0.12515 1.52402

D6 -2.68941 0.00007 -0.00681 -0.10629 -0.11314 -2.80256

D7 -3.10317 -0.00010 0.00208 -0.03925 -0.03718 -3.14035

D8 0.00367 0.00003 -0.00181 0.00665 0.00486 0.00852

D9 -3.11917 -0.00003 0.00079 -0.02722 -0.02646 3.13755

D10 -1.04618 -0.00005 0.00085 -0.03176 -0.03095 -1.07713

D11 1.06431 -0.00007 0.00085 -0.03820 -0.03740 1.02691

D12 1.06152 -0.00003 0.00037 -0.03069 -0.03029 1.03122

D13 3.13451 -0.00006 0.00043 -0.03523 -0.03478 3.09973

D14 -1.03819 -0.00008 0.00043 -0.04167 -0.04123 -1.07942

D15 -0.97631 0.00005 0.00175 -0.04848 -0.04670 -1.02302

D16 1.09668 0.00003 0.00181 -0.05301 -0.05119 1.04549

D17 -3.07602 0.00001 0.00181 -0.05946 -0.05764 -3.13366

D18 3.13629 0.00025 0.01536 -0.06463 -0.04928 3.08701

D19 -0.93874 0.00027 0.01537 -0.07812 -0.06276 -1.00150

D20 1.16375 0.00020 0.01470 -0.06749 -0.05278 1.11097

D21 1.84647 -0.00030 -0.00339 0.00426 0.00081 1.84728

D22 -1.11448 0.00022 -0.00093 0.05568 0.05481 -1.05967

D23 2.55037 0.00028 0.00850 -0.03107 -0.02273 2.52764

D24 -0.77332 -0.00023 0.00593 -0.08132 -0.07523 -0.84856

D25 -2.99355 -0.00014 -0.01426 -0.23357 -0.24779 3.04184

D26 -0.87641 -0.00015 -0.01383 -0.23535 -0.24921 -1.12562

D27 1.15972 -0.00002 -0.01375 -0.22379 -0.23754 0.92218

D28 -3.10325 0.00002 -0.00202 -0.06473 -0.06677 3.11317

D29 -0.98307 0.00006 -0.00198 -0.05610 -0.05811 -1.04118

D30 1.05626 0.00004 -0.00237 -0.06259 -0.06497 0.99129

D31 1.10120 -0.00004 -0.00249 -0.06428 -0.06676 1.03444

D32 -3.06181 0.00000 -0.00245 -0.05565 -0.05810 -3.11992

D33 -1.02248 -0.00002 -0.00284 -0.06214 -0.06497 -1.08744

D34 -0.99901 -0.00014 -0.00287 -0.07458 -0.07743 -1.07644

D35 1.12117 -0.00010 -0.00283 -0.06594 -0.06877 1.05240

D36 -3.12268 -0.00012 -0.00322 -0.07243 -0.07563 3.08487

D37 -3.12790 -0.00002 -0.00567 0.06380 0.05815 -3.06975

D38 -0.99709 -0.00005 -0.00514 0.05242 0.04730 -0.94980

D39 1.02445 0.00000 -0.00527 0.05865 0.05341 1.07786

D40 1.02825 0.00002 -0.00544 0.05979 0.05433 1.08257

D41 -3.12414 -0.00001 -0.00491 0.04840 0.04348 -3.08066

D42 -1.10259 0.00003 -0.00504 0.05463 0.04959 -1.05301

D43 -1.00128 0.00003 -0.00515 0.06346 0.05829 -0.94299

D44 1.12952 0.00000 -0.00463 0.05207 0.04744 1.17696

D45 -3.13212 0.00005 -0.00475 0.05830 0.05355 -3.07857

D46 -3.13907 -0.00003 -0.00117 -0.02090 -0.02206 3.12205

D47 -1.04454 -0.00002 -0.00114 -0.01879 -0.01992 -1.06446

D48 1.04798 -0.00002 -0.00118 -0.01937 -0.02053 1.02745

D49 1.01692 0.00001 -0.00170 -0.01049 -0.01220 1.00472

D50 3.11145 0.00002 -0.00166 -0.00839 -0.01006 3.10139

D51 -1.07921 0.00002 -0.00170 -0.00896 -0.01067 -1.08988

D52 -1.01154 -0.00002 -0.00143 -0.01305 -0.01448 -1.02602

D53 1.08299 0.00000 -0.00140 -0.01095 -0.01234 1.07065

D54 -3.10768 -0.00001 -0.00143 -0.01152 -0.01295 -3.12062

Item Value Threshold Converged?

Maximum Force 0.000617 0.000450 NO

RMS Force 0.000135 0.000300 YES

Maximum Displacement 0.621063 0.001800 NO

RMS Displacement 0.184652 0.001200 NO

Predicted change in Energy=-7.617887D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:41:54 2019, MaxMem= 1342177280 cpu: 0.6

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.134271 -0.346792 -0.130192

2 6 0 -2.827016 0.036788 0.510899

3 8 0 -4.998446 0.434618 -0.461499

4 8 0 -4.266089 -1.683331 -0.300474

5 6 0 -2.334087 -0.926941 1.575295

6 16 0 -1.582196 0.220951 -0.919712

7 6 0 -0.109177 0.757369 -0.113605

8 16 0 1.126742 -0.533931 -0.002183

9 16 0 -0.014181 2.224726 0.785026

10 6 0 2.712605 0.372095 -0.196005

11 6 0 3.873594 -0.594402 0.021158

12 6 0 5.240170 0.072460 -0.161885

13 6 0 6.392428 -0.925224 -0.041545

14 1 0 -2.952638 1.039063 0.916880

15 1 0 -5.128071 -1.853104 -0.717703

16 1 0 -1.384871 -0.575176 1.980499

17 1 0 -3.053811 -0.975037 2.400096

18 1 0 -2.195482 -1.934934 1.181774

19 1 0 2.734184 0.801311 -1.201887

20 1 0 2.739665 1.188679 0.526798

21 1 0 3.810609 -1.023337 1.029385

22 1 0 3.788195 -1.433563 -0.680005

23 1 0 5.276376 0.553738 -1.146844

24 1 0 5.363616 0.873098 0.577943

25 1 0 7.362848 -0.441510 -0.193531

26 1 0 6.410380 -1.395760 0.947758

27 1 0 6.301083 -1.723491 -0.786216

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.505671 0.000000

3 O 1.211265 2.412247 0.000000

4 O 1.353776 2.384967 2.246772 0.000000

5 C 2.546748 1.518121 3.619556 2.797011 0.000000

6 S 2.731073 1.905292 3.453459 3.348586 2.847464

7 C 4.173827 2.880259 4.912245 4.824091 3.261826

8 S 5.265896 4.027552 6.218278 5.522021 3.823641

9 S 4.942214 3.574110 5.440700 5.876219 3.992430

10 C 6.884827 5.594600 7.715874 7.275841 5.504007

11 C 8.013121 6.748068 8.944547 8.218494 6.407903

12 C 9.383865 8.095271 10.249399 9.668039 7.834920

13 C 10.542952 9.285947 11.479440 10.688580 8.875034

14 H 2.100764 1.088649 2.539805 3.258609 2.163628

15 H 1.897837 3.221181 2.305670 0.972583 3.731216

16 H 3.473669 2.148024 4.476713 3.838262 1.090384

17 H 2.822135 2.155062 3.735969 3.043744 1.095725

18 H 2.828843 2.176372 4.021409 2.558862 1.090926

19 H 7.045733 5.868993 7.776645 7.482634 6.032161

20 H 7.073917 5.684632 7.837328 7.616653 5.596262

21 H 8.057509 6.741718 9.052503 8.212013 6.169651

22 H 8.015537 6.880494 8.985705 8.067088 6.544110

23 H 9.508145 8.287359 10.298342 9.837655 8.217152

24 H 9.602054 8.233491 10.423293 10.001908 7.968029

25 H 11.497684 10.225377 12.395201 11.695543 9.868887

26 H 10.651384 9.358020 11.640344 10.753035 8.779481

27 H 10.546197 9.386335 11.508355 10.578406 8.987624

6 7 8 9 10

6 S 0.000000

7 C 1.762764 0.000000

8 S 2.958048 1.790912 0.000000

9 S 3.062666 1.723282 3.087328 0.000000

10 C 4.357971 2.849154 1.836685 3.439480 0.000000

11 C 5.596041 4.208076 2.747616 4.862691 1.526162

12 C 6.865933 5.393231 4.160950 5.756483 2.545492

13 C 8.104290 6.716187 5.280351 7.186796 3.904867

14 H 2.433205 3.037519 4.467698 3.171390 5.811914

15 H 4.112875 5.689359 6.432331 6.711093 8.167000

16 H 3.013963 2.790760 3.200145 3.338772 4.735378

17 H 3.823240 4.241556 4.841750 4.699605 6.465761

18 H 3.072490 3.644059 3.794961 4.713624 5.595532

19 H 4.364353 3.044830 2.409571 3.677967 1.093842

20 H 4.659117 2.951617 2.418414 2.953598 1.090864

21 H 5.867672 4.454442 2.916641 5.023807 2.157411

22 H 5.624586 4.506717 2.890002 5.476081 2.156746

23 H 6.870396 5.487552 4.439903 5.874889 2.740440

24 H 7.135305 5.517526 4.501931 5.548917 2.806752

25 H 8.998889 7.568015 6.239726 7.904868 4.720881

26 H 8.365553 6.947451 5.437092 7.376272 4.255237

27 H 8.120638 6.906410 5.366895 7.611818 4.197261

11 12 13 14 15

11 C 0.000000

12 C 1.531581 0.000000

13 C 2.541240 1.528906 0.000000

14 H 7.075872 8.319866 9.597253 0.000000

15 H 9.119223 10.560169 11.577567 3.971020 0.000000

16 H 5.611670 6.992883 8.043480 2.488965 4.788000

17 H 7.334382 8.743633 9.756819 2.503351 3.846327

18 H 6.322795 7.818182 8.733167 3.080277 3.494966

19 H 2.177638 2.809411 4.208332 6.073356 8.312365

20 H 2.172750 2.823607 4.258436 5.707615 8.526576

21 H 1.097486 2.159524 2.796839 7.071609 9.145536

22 H 1.096866 2.155177 2.729115 7.355457 8.926211

23 H 2.156444 1.096851 2.157449 8.497716 10.687824

24 H 2.164193 1.097089 2.162448 8.324813 10.917252

25 H 3.499195 2.184246 1.094895 10.480189 12.581352

26 H 2.817100 2.180911 1.095649 9.674473 11.666996

27 H 2.796319 2.177330 1.095495 9.806304 11.430095

16 17 18 19 20

16 H 0.000000

17 H 1.766723 0.000000

18 H 1.773131 1.772693 0.000000

19 H 5.384135 7.044898 6.121314 0.000000

20 H 4.715531 6.461832 5.877212 1.771563 0.000000

21 H 5.300799 7.000102 6.076788 3.076785 2.508491

22 H 5.880113 7.517334 6.286651 2.525463 3.071147

23 H 7.444927 9.182045 8.212466 2.554811 3.104695

24 H 7.043205 8.808457 8.086385 3.175981 2.643355

25 H 9.014814 10.747946 9.771563 4.897542 4.954817

26 H 7.906064 9.584216 8.625910 4.791921 4.508956

27 H 8.249074 9.910944 8.724065 4.389781 4.784186

21 22 23 24 25

21 H 0.000000

22 H 1.758068 0.000000

23 H 3.061309 2.526259 0.000000

24 H 2.492408 3.063507 1.756272 0.000000

25 H 3.801638 3.741520 2.500538 2.514020 0.000000

26 H 2.627580 3.086567 3.077964 2.525905 1.766445

27 H 3.160552 2.531787 2.523063 3.079294 1.766946

26 27

26 H 0.000000

27 H 1.768055 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 6.29D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.136487 -0.407312 -0.111958

2 6 0 -2.829786 0.072607 0.461850

3 8 0 -5.001185 0.312182 -0.561166

4 8 0 -4.267137 -1.754176 -0.071958

5 6 0 -2.336452 -0.713089 1.663514

6 16 0 -1.584591 0.032720 -0.979690

7 6 0 -0.112313 0.689466 -0.266655

8 16 0 1.124631 -0.567626 0.044882

9 16 0 -0.018861 2.278994 0.392412

10 6 0 2.709817 0.298525 -0.287358

11 6 0 3.871523 -0.621322 0.078006

12 6 0 5.237616 0.010073 -0.206377

13 6 0 6.390653 -0.955673 0.068203

14 1 0 -2.956386 1.125784 0.706690

15 1 0 -5.128825 -1.987632 -0.457845

16 1 0 -1.387677 -0.301660 2.009187

17 1 0 -3.056440 -0.632724 2.485567

18 1 0 -2.196869 -1.769962 1.431875

19 1 0 2.731412 0.565802 -1.347824

20 1 0 2.735936 1.217772 0.299401

21 1 0 3.808521 -0.887992 1.140735

22 1 0 3.787077 -1.559551 -0.483874

23 1 0 5.273787 0.332048 -1.254283

24 1 0 5.360128 0.916306 0.399706

25 1 0 7.360729 -0.500697 -0.157060

26 1 0 6.408630 -1.266314 1.118740

27 1 0 6.300242 -1.860290 -0.543026

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3418356 0.1906765 0.1786081

Leave Link 202 at Sat Aug 17 17:41:54 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1099.1191431824 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0545980032 Hartrees.

Nuclear repulsion after empirical dispersion term = 1099.0645451792 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2324

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.40D-09

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 103

GePol: Fraction of low-weight points (<1% of avg) = 4.43%

GePol: Cavity surface area = 310.176 Ang\*\*2

GePol: Cavity volume = 321.267 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0055132466 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1099.0590319325 Hartrees.

Leave Link 301 at Sat Aug 17 17:41:54 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.88D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:41:54 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:41:54 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999965 -0.008256 -0.000596 -0.000741 Ang= -0.95 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.62752224760

Leave Link 401 at Sat Aug 17 17:41:55 2019, MaxMem= 1342177280 cpu: 7.5

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16202928.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.33D-15 for 2300.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.40D-15 for 837 731.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.00D-15 for 2299.

Iteration 1 A^-1\*A deviation from orthogonality is 1.29D-13 for 888 863.

E= -1658.57741746817

DIIS: error= 1.15D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.57741746817 IErMin= 1 ErrMin= 1.15D-02

ErrMax= 1.15D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.19D-01 BMatP= 2.19D-01

IDIUse=3 WtCom= 8.85D-01 WtEn= 1.15D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Recover alternate guess density for next cycle.

RMSDP=2.27D-03 MaxDP=7.62D-02 OVMax= 0.00D+00

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.27D-03 CP: 9.97D-01

E= -1658.22331131063 Delta-E= 0.354106157539 Rises=F Damp=F

Switch densities from cycles 1 and 2 for lowest energy.

DIIS: error= 3.41D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 1 EnMin= -1658.57741746817 IErMin= 1 ErrMin= 1.15D-02

ErrMax= 3.41D-02 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.18D+00 BMatP= 2.19D-01

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.917D+00 0.833D-01

Coeff: 0.917D+00 0.833D-01

Gap= 0.117 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=1.38D-02 MaxDP=5.41D-01 DE= 3.54D-01 OVMax= 1.68D-01

Cycle 3 Pass 1 IDiag 1:

RMSU= 9.16D-04 CP: 9.97D-01 1.10D-01

E= -1658.66807465916 Delta-E= -0.444763348531 Rises=F Damp=F

DIIS: error= 4.29D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.66807465916 IErMin= 3 ErrMin= 4.29D-03

ErrMax= 4.29D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.72D-02 BMatP= 2.19D-01

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.239D-01 0.107D+00 0.917D+00

Coeff: -0.239D-01 0.107D+00 0.917D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=3.32D-04 MaxDP=1.75D-02 DE=-4.45D-01 OVMax= 2.26D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.33D-04 CP: 9.97D-01 2.10D-01 9.35D-01

E= -1658.67413038316 Delta-E= -0.006055723996 Rises=F Damp=F

DIIS: error= 3.35D-03 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67413038316 IErMin= 4 ErrMin= 3.35D-03

ErrMax= 3.35D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.13D-02 BMatP= 3.72D-02

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.316D-01 0.454D-01 0.509D+00 0.477D+00

Coeff: -0.316D-01 0.454D-01 0.509D+00 0.477D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.57D-04 MaxDP=8.12D-03 DE=-6.06D-03 OVMax= 1.63D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 9.57D-05 CP: 9.97D-01 2.04D-01 9.70D-01 4.91D-01

E= -1658.67592738711 Delta-E= -0.001797003951 Rises=F Damp=F

DIIS: error= 1.62D-03 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67592738711 IErMin= 5 ErrMin= 1.62D-03

ErrMax= 1.62D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.79D-03 BMatP= 1.13D-02

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.112D-01 0.547D-02 0.140D+00 0.307D+00 0.558D+00

Coeff: -0.112D-01 0.547D-02 0.140D+00 0.307D+00 0.558D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.03D-05 MaxDP=2.73D-03 DE=-1.80D-03 OVMax= 5.82D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.59D-05 CP: 9.97D-01 2.01D-01 9.73D-01 6.17D-01 6.11D-01

E= -1658.67628188874 Delta-E= -0.000354501628 Rises=F Damp=F

DIIS: error= 2.99D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67628188874 IErMin= 6 ErrMin= 2.99D-04

ErrMax= 2.99D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 8.13D-05 BMatP= 1.79D-03

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.411D-02 0.795D-03 0.471D-01 0.135D+00 0.292D+00 0.529D+00

Coeff: -0.411D-02 0.795D-03 0.471D-01 0.135D+00 0.292D+00 0.529D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.41D-05 MaxDP=5.91D-04 DE=-3.55D-04 OVMax= 1.40D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.01D-05 CP: 9.97D-01 2.00D-01 9.74D-01 6.41D-01 6.64D-01

CP: 8.54D-01

E= -1658.67629806481 Delta-E= -0.000016176074 Rises=F Damp=F

DIIS: error= 8.02D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67629806481 IErMin= 7 ErrMin= 8.02D-05

ErrMax= 8.02D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 6.77D-06 BMatP= 8.13D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.552D-03-0.418D-03 0.277D-02 0.240D-01 0.667D-01 0.241D+00

Coeff-Com: 0.666D+00

Coeff: -0.552D-03-0.418D-03 0.277D-02 0.240D-01 0.667D-01 0.241D+00

Coeff: 0.666D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.60D-06 MaxDP=1.87D-04 DE=-1.62D-05 OVMax= 5.60D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 4.44D-06 CP: 9.97D-01 1.99D-01 9.74D-01 6.49D-01 6.90D-01

CP: 8.89D-01 9.72D-01

E= -1658.67629968823 Delta-E= -0.000001623419 Rises=F Damp=F

DIIS: error= 2.55D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67629968823 IErMin= 8 ErrMin= 2.55D-05

ErrMax= 2.55D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.36D-06 BMatP= 6.77D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.180D-03-0.346D-03-0.413D-02-0.223D-02 0.368D-02 0.650D-01

Coeff-Com: 0.339D+00 0.598D+00

Coeff: 0.180D-03-0.346D-03-0.413D-02-0.223D-02 0.368D-02 0.650D-01

Coeff: 0.339D+00 0.598D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.90D-06 MaxDP=1.72D-04 DE=-1.62D-06 OVMax= 5.77D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.20D-06 CP: 9.97D-01 1.99D-01 9.74D-01 6.54D-01 6.90D-01

CP: 9.55D-01 1.15D+00 9.51D-01

E= -1658.67630010895 Delta-E= -0.000000420712 Rises=F Damp=F

DIIS: error= 1.32D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67630010895 IErMin= 9 ErrMin= 1.32D-05

ErrMax= 1.32D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.51D-07 BMatP= 1.36D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.232D-03-0.691D-04-0.276D-02-0.704D-02-0.139D-01-0.235D-01

Coeff-Com: -0.392D-02 0.274D+00 0.777D+00

Coeff: 0.232D-03-0.691D-04-0.276D-02-0.704D-02-0.139D-01-0.235D-01

Coeff: -0.392D-02 0.274D+00 0.777D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.89D-06 MaxDP=1.08D-04 DE=-4.21D-07 OVMax= 3.12D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 9.40D-07 CP: 9.97D-01 1.99D-01 9.74D-01 6.56D-01 6.96D-01

CP: 9.77D-01 1.22D+00 1.16D+00 9.39D-01

E= -1658.67630021660 Delta-E= -0.000000107657 Rises=F Damp=F

DIIS: error= 7.08D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67630021660 IErMin=10 ErrMin= 7.08D-06

ErrMax= 7.08D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.27D-07 BMatP= 2.51D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.122D-03 0.457D-04-0.944D-03-0.464D-02-0.112D-01-0.327D-01

Coeff-Com: -0.842D-01 0.464D-01 0.530D+00 0.557D+00

Coeff: 0.122D-03 0.457D-04-0.944D-03-0.464D-02-0.112D-01-0.327D-01

Coeff: -0.842D-01 0.464D-01 0.530D+00 0.557D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.26D-06 MaxDP=5.95D-05 DE=-1.08D-07 OVMax= 1.99D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 3.95D-07 CP: 9.97D-01 1.99D-01 9.74D-01 6.58D-01 6.97D-01

CP: 9.90D-01 1.28D+00 1.26D+00 1.23D+00 7.99D-01

E= -1658.67630025632 Delta-E= -0.000000039716 Rises=F Damp=F

DIIS: error= 2.03D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67630025632 IErMin=11 ErrMin= 2.03D-06

ErrMax= 2.03D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 9.18D-09 BMatP= 1.27D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.177D-04 0.289D-04 0.607D-04-0.779D-03-0.233D-02-0.966D-02

Coeff-Com: -0.346D-01-0.270D-01 0.104D+00 0.239D+00 0.731D+00

Coeff: 0.177D-04 0.289D-04 0.607D-04-0.779D-03-0.233D-02-0.966D-02

Coeff: -0.346D-01-0.270D-01 0.104D+00 0.239D+00 0.731D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.26D-07 MaxDP=2.00D-05 DE=-3.97D-08 OVMax= 5.60D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.69D-07 CP: 9.97D-01 1.99D-01 9.74D-01 6.59D-01 6.98D-01

CP: 9.92D-01 1.29D+00 1.29D+00 1.27D+00 9.52D-01

CP: 9.02D-01

E= -1658.67630025996 Delta-E= -0.000000003643 Rises=F Damp=F

DIIS: error= 1.15D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.67630025996 IErMin=12 ErrMin= 1.15D-06

ErrMax= 1.15D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.51D-09 BMatP= 9.18D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.159D-04 0.417D-05 0.230D-03 0.573D-03 0.110D-02 0.147D-02

Coeff-Com: -0.730D-03-0.227D-01-0.549D-01-0.137D-01 0.378D+00 0.711D+00

Coeff: -0.159D-04 0.417D-05 0.230D-03 0.573D-03 0.110D-02 0.147D-02

Coeff: -0.730D-03-0.227D-01-0.549D-01-0.137D-01 0.378D+00 0.711D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.72D-07 MaxDP=8.15D-06 DE=-3.64D-09 OVMax= 1.75D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 7.05D-08 CP: 9.97D-01 1.99D-01 9.74D-01 6.59D-01 6.98D-01

CP: 9.94D-01 1.29D+00 1.30D+00 1.31D+00 9.87D-01

CP: 1.11D+00 9.44D-01

E= -1658.67630026085 Delta-E= -0.000000000889 Rises=F Damp=F

DIIS: error= 2.86D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1658.67630026085 IErMin=13 ErrMin= 2.86D-07

ErrMax= 2.86D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.41D-10 BMatP= 2.51D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.701D-05-0.209D-05 0.647D-04 0.275D-03 0.590D-03 0.152D-02

Coeff-Com: 0.392D-02-0.366D-02-0.275D-01-0.351D-01 0.470D-01 0.230D+00

Coeff-Com: 0.782D+00

Coeff: -0.701D-05-0.209D-05 0.647D-04 0.275D-03 0.590D-03 0.152D-02

Coeff: 0.392D-02-0.366D-02-0.275D-01-0.351D-01 0.470D-01 0.230D+00

Coeff: 0.782D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.34D-08 MaxDP=2.21D-06 DE=-8.89D-10 OVMax= 6.55D-06

Cycle 14 Pass 1 IDiag 1:

RMSU= 2.16D-08 CP: 9.97D-01 1.99D-01 9.74D-01 6.59D-01 6.97D-01

CP: 9.94D-01 1.29D+00 1.30D+00 1.31D+00 1.00D+00

CP: 1.16D+00 1.09D+00 9.90D-01

E= -1658.67630026090 Delta-E= -0.000000000046 Rises=F Damp=F

DIIS: error= 8.71D-08 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1658.67630026090 IErMin=14 ErrMin= 8.71D-08

ErrMax= 8.71D-08 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.86D-11 BMatP= 1.41D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.219D-06-0.894D-06-0.148D-04-0.417D-05 0.517D-05 0.219D-03

Coeff-Com: 0.116D-02 0.179D-02 0.611D-03-0.872D-02-0.368D-01-0.410D-01

Coeff-Com: 0.213D+00 0.870D+00

Coeff: 0.219D-06-0.894D-06-0.148D-04-0.417D-05 0.517D-05 0.219D-03

Coeff: 0.116D-02 0.179D-02 0.611D-03-0.872D-02-0.368D-01-0.410D-01

Coeff: 0.213D+00 0.870D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.95D-08 MaxDP=1.18D-06 DE=-4.59D-11 OVMax= 2.30D-06

Cycle 15 Pass 1 IDiag 1:

RMSU= 8.27D-09 CP: 9.97D-01 1.99D-01 9.74D-01 6.59D-01 6.97D-01

CP: 9.94D-01 1.29D+00 1.30D+00 1.31D+00 1.00D+00

CP: 1.18D+00 1.14D+00 1.17D+00 1.04D+00

E= -1658.67630026089 Delta-E= 0.000000000006 Rises=F Damp=F

DIIS: error= 5.01D-08 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=14 EnMin= -1658.67630026090 IErMin=15 ErrMin= 5.01D-08

ErrMax= 5.01D-08 0.00D+00 EMaxC= 1.00D+00 BMatC= 4.96D-12 BMatP= 1.86D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D-05-0.125D-06-0.152D-04-0.372D-04-0.756D-04-0.106D-03

Coeff-Com: -0.679D-04 0.120D-02 0.464D-02 0.978D-03-0.230D-01-0.533D-01

Coeff-Com: -0.781D-02 0.426D+00 0.651D+00

Coeff: 0.100D-05-0.125D-06-0.152D-04-0.372D-04-0.756D-04-0.106D-03

Coeff: -0.679D-04 0.120D-02 0.464D-02 0.978D-03-0.230D-01-0.533D-01

Coeff: -0.781D-02 0.426D+00 0.651D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.41D-09 MaxDP=4.35D-07 DE= 6.37D-12 OVMax= 1.10D-06

Error on total polarization charges = 0.04189

SCF Done: E(UB3LYP) = -1658.67630026 A.U. after 15 cycles

NFock= 15 Conv=0.64D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7553 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655194195061D+03 PE=-6.140848113970D+03 EE= 1.727918586715D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.46

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7553, after 0.7500

Leave Link 502 at Sat Aug 17 17:42:25 2019, MaxMem= 1342177280 cpu: 357.1

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 338

Leave Link 701 at Sat Aug 17 17:42:26 2019, MaxMem= 1342177280 cpu: 10.2

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:42:26 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:42:29 2019, MaxMem= 1342177280 cpu: 35.9

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.34764690D+00-2.99618940D+00 4.41927358D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.003212048 -0.000383082 0.002956645

2 6 0.000113276 -0.001616378 -0.002349040

3 8 0.002269066 -0.001479037 -0.001080154

4 8 0.000963313 0.001560737 -0.000585802

5 6 -0.000261119 -0.000179056 0.000215271

6 16 -0.000338455 0.000774028 0.001038877

7 6 -0.001227358 -0.000160303 0.001851364

8 16 -0.001013361 -0.000922339 0.000608212

9 16 -0.000523602 0.000227125 -0.001388602

10 6 0.000918892 -0.000194487 -0.000106921

11 6 0.000102995 0.000008980 -0.000150260

12 6 0.000339331 -0.000158598 -0.000995499

13 6 0.000285406 0.000425523 0.000485278

14 1 0.000283641 0.000130130 -0.000512487

15 1 0.000553044 0.001523819 0.000067706

16 1 0.000581498 0.000075920 0.000181398

17 1 0.000406584 -0.000211823 -0.000081661

18 1 0.000396607 0.000786705 -0.000220148

19 1 0.000698543 -0.000048553 0.000750364

20 1 -0.000791184 -0.000396946 0.000092739

21 1 -0.000009892 0.000287924 -0.000872791

22 1 0.000391875 0.000159585 0.000157702

23 1 0.000158626 -0.000014535 0.000242593

24 1 -0.000568966 -0.000440203 -0.000403146

25 1 -0.000526700 -0.000025308 0.000128403

26 1 -0.000164455 0.000054094 -0.000475862

27 1 0.000174442 0.000216077 0.000445819

-------------------------------------------------------------------

Cartesian Forces: Max 0.003212048 RMS 0.000877793

Leave Link 716 at Sat Aug 17 17:42:29 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.003159569 RMS 0.000922122

Search for a local minimum.

Step number 28 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .92212D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 3 4 5 6

2 8 9 10 11

12 13 17 27 28

DE= 6.76D-04 DEPred=-7.62D-05 R=-8.87D+00

Trust test=-8.87D+00 RLast= 6.43D-01 DXMaxT set to 5.00D-02

ITU= -1 0 0 -1 0 0 -1 1 -1 1 -1 1 1 -1 1 -1 1 1 -1 0

ITU= 0 -1 0 0 -1 -1 0 0

Eigenvalues --- 0.00000 0.00170 0.00210 0.00253 0.00397

Eigenvalues --- 0.00453 0.00515 0.00728 0.01098 0.02291

Eigenvalues --- 0.02437 0.03530 0.03606 0.03874 0.04540

Eigenvalues --- 0.04666 0.04810 0.04987 0.05194 0.05453

Eigenvalues --- 0.05508 0.05542 0.05667 0.05851 0.08019

Eigenvalues --- 0.08285 0.08356 0.11150 0.11737 0.12185

Eigenvalues --- 0.13218 0.14869 0.15552 0.15981 0.16008

Eigenvalues --- 0.16081 0.16203 0.16241 0.16716 0.17316

Eigenvalues --- 0.18872 0.21079 0.21913 0.22114 0.22669

Eigenvalues --- 0.23692 0.24449 0.25304 0.25546 0.26411

Eigenvalues --- 0.26973 0.27832 0.29066 0.29400 0.29623

Eigenvalues --- 0.29944 0.30276 0.32036 0.33680 0.33872

Eigenvalues --- 0.33881 0.33942 0.33968 0.34036 0.34047

Eigenvalues --- 0.34111 0.34158 0.34354 0.34514 0.34580

Eigenvalues --- 0.34671 0.36679 0.52450 0.55944 1.01893

Eigenvalue 1 is 4.20D-08 Eigenvector:

D4 D6 D1 D5 D3

1 0.38516 0.37264 0.36821 0.36156 0.35569

D2 D20 D18 D19 D22

1 0.34461 0.22031 0.21013 0.19757 -0.08005

En-DIIS/RFO-DIIS IScMMF= 0 using points: 28 27 26

RFO step: Lambda=-2.47238939D-04.

NNeg= 0 NP= 3 Switch= 2.50D-03 Rises=T DC= 5.57D-06 SmlDif= 1.00D-05

RMS Error= 0.3104556551D-02 NUsed= 3 EDIIS=F

DidBck=T Rises=T RFO-DIIS coefs: 0.09374 -0.81348 1.71975

Iteration 1 RMS(Cart)= 0.20132756 RMS(Int)= 0.07128375

Iteration 2 RMS(Cart)= 0.08796364 RMS(Int)= 0.02443840

Iteration 3 RMS(Cart)= 0.03428719 RMS(Int)= 0.00157870

Iteration 4 RMS(Cart)= 0.00175772 RMS(Int)= 0.00049644

Iteration 5 RMS(Cart)= 0.00000376 RMS(Int)= 0.00049643

Iteration 6 RMS(Cart)= 0.00000000 RMS(Int)= 0.00049643

ITry= 1 IFail=0 DXMaxC= 1.32D+00 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.84531 -0.00139 -0.00895 0.00467 -0.00428 2.84102

R2 2.28896 -0.00227 -0.00321 -0.01043 -0.01364 2.27532

R3 2.55827 -0.00316 -0.00594 0.00165 -0.00429 2.55398

R4 2.86883 0.00012 -0.00234 -0.00900 -0.01134 2.85749

R5 3.60048 -0.00246 -0.00347 0.03870 0.03523 3.63571

R6 2.05725 -0.00010 -0.00021 0.00007 -0.00014 2.05710

R7 1.83792 -0.00078 -0.00191 -0.00285 -0.00476 1.83316

R8 2.06053 0.00060 0.00017 -0.00389 -0.00372 2.05680

R9 2.07062 -0.00032 -0.00241 -0.00304 -0.00545 2.06517

R10 2.06155 -0.00060 -0.00183 -0.00065 -0.00249 2.05906

R11 3.33114 -0.00161 -0.01031 -0.02254 -0.03284 3.29830

R12 3.38433 0.00081 0.00080 -0.00462 -0.00381 3.38052

R13 3.25653 -0.00055 -0.00325 0.00104 -0.00221 3.25432

R14 3.47083 0.00084 0.00325 0.00324 0.00649 3.47733

R15 2.88403 -0.00035 -0.00343 -0.00366 -0.00709 2.87694

R16 2.06706 -0.00070 -0.00384 -0.00180 -0.00564 2.06142

R17 2.06143 -0.00025 -0.00198 -0.00156 -0.00354 2.05789

R18 2.89427 -0.00021 -0.00060 -0.00082 -0.00142 2.89285

R19 2.07395 -0.00091 -0.00216 -0.00084 -0.00300 2.07095

R20 2.07278 -0.00025 -0.00232 -0.00069 -0.00301 2.06977

R21 2.88921 -0.00054 -0.00357 -0.00308 -0.00665 2.88256

R22 2.07275 -0.00022 -0.00135 -0.00057 -0.00191 2.07083

R23 2.07320 -0.00066 -0.00198 -0.00092 -0.00290 2.07030

R24 2.06905 -0.00050 -0.00193 -0.00071 -0.00265 2.06640

R25 2.07048 -0.00045 -0.00188 -0.00095 -0.00283 2.06764

R26 2.07018 -0.00046 -0.00175 -0.00062 -0.00237 2.06782

A1 2.17918 0.00002 -0.00077 -0.01061 -0.01111 2.16808

A2 1.97100 0.00039 0.00261 0.00446 0.00734 1.97835

A3 2.13298 -0.00040 -0.00256 0.00598 0.00369 2.13667

A4 2.00282 0.00203 0.01840 0.02075 0.03873 2.04156

A5 1.84644 -0.00025 -0.00666 -0.05756 -0.06399 1.78245

A6 1.86831 -0.00087 0.00405 0.00021 0.00407 1.87238

A7 1.95592 -0.00135 -0.00964 0.00378 -0.00543 1.95048

A8 1.93955 0.00007 0.00075 -0.00022 0.00026 1.93981

A9 1.84047 0.00024 -0.00917 0.03210 0.02290 1.86337

A10 1.88872 -0.00259 -0.01524 -0.00258 -0.01782 1.87090

A11 1.91603 0.00003 -0.00381 0.00641 0.00259 1.91862

A12 1.92022 0.00069 0.00820 -0.00342 0.00477 1.92499

A13 1.95508 -0.00064 -0.00282 0.00394 0.00114 1.95622

A14 1.88203 -0.00019 0.00124 0.00272 0.00393 1.88596

A15 1.89814 -0.00004 -0.00443 -0.00009 -0.00448 1.89366

A16 1.89065 0.00015 0.00164 -0.00974 -0.00809 1.88256

A17 1.80493 -0.00309 -0.01173 0.03768 0.02595 1.83088

A18 1.96678 0.00033 0.00189 0.02205 0.02085 1.98762

A19 2.14557 -0.00148 -0.00286 0.00117 -0.00480 2.14076

A20 2.14535 0.00154 0.00960 -0.00056 0.00595 2.15130

A21 1.80659 -0.00255 -0.01084 -0.00146 -0.01230 1.79430

A22 1.90649 0.00314 0.01912 0.01028 0.02937 1.93586

A23 1.88351 -0.00019 -0.00728 -0.00030 -0.00776 1.87575

A24 1.89733 -0.00193 -0.00275 -0.01096 -0.01367 1.88366

A25 1.94372 -0.00138 -0.00398 0.00571 0.00167 1.94539

A26 1.94003 -0.00002 -0.00134 -0.00351 -0.00476 1.93528

A27 1.89135 0.00032 -0.00427 -0.00166 -0.00596 1.88539

A28 1.96711 -0.00150 -0.01308 -0.00427 -0.01735 1.94977

A29 1.91195 0.00008 0.00489 -0.00212 0.00274 1.91469

A30 1.91167 0.00102 0.00384 0.00781 0.01166 1.92333

A31 1.90834 0.00052 -0.00188 0.00116 -0.00075 1.90759

A32 1.90306 0.00021 0.00652 0.00149 0.00805 1.91111

A33 1.85853 -0.00025 0.00043 -0.00405 -0.00363 1.85490

A34 1.95943 0.00083 0.00687 0.00232 0.00914 1.96857

A35 1.90479 0.00004 0.00204 0.00445 0.00642 1.91121

A36 1.91512 -0.00073 -0.00749 -0.00401 -0.01149 1.90363

A37 1.90936 -0.00008 0.00369 0.00299 0.00661 1.91597

A38 1.91595 -0.00021 -0.00336 -0.00102 -0.00436 1.91159

A39 1.85629 0.00011 -0.00224 -0.00507 -0.00729 1.84900

A40 1.94846 -0.00029 -0.00283 0.00322 0.00039 1.94886

A41 1.94299 -0.00006 -0.00044 0.00149 0.00105 1.94404

A42 1.93816 0.00035 0.00539 0.00260 0.00798 1.94614

A43 1.87606 0.00016 0.00026 -0.00096 -0.00070 1.87536

A44 1.87703 0.00003 -0.00028 -0.00444 -0.00473 1.87230

A45 1.87780 -0.00019 -0.00224 -0.00240 -0.00465 1.87316

D1 2.49253 0.00140 0.15423 0.37838 0.53284 3.02537

D2 -1.62508 0.00081 0.14882 0.35372 0.50223 -1.12285

D3 0.33153 0.00060 0.13723 0.36444 0.50166 0.83319

D4 -0.64156 -0.00038 0.10826 0.40212 0.51068 -0.13088

D5 1.52402 -0.00098 0.10285 0.37746 0.48007 2.00408

D6 -2.80256 -0.00119 0.09126 0.38819 0.47949 -2.32306

D7 -3.14035 0.00112 0.03714 0.01017 0.04742 -3.09293

D8 0.00852 -0.00061 -0.00740 0.03328 0.02578 0.03430

D9 3.13755 -0.00021 0.02528 -0.05554 -0.03038 3.10717

D10 -1.07713 0.00000 0.02945 -0.05038 -0.02102 -1.09815

D11 1.02691 0.00024 0.03530 -0.06244 -0.02724 0.99967

D12 1.03122 -0.00034 0.02806 0.00259 0.03067 1.06189

D13 3.09973 -0.00013 0.03223 0.00776 0.04003 3.13976

D14 -1.07942 0.00011 0.03807 -0.00430 0.03381 -1.04561

D15 -1.02302 0.00019 0.04523 -0.04014 0.00515 -1.01787

D16 1.04549 0.00041 0.04939 -0.03497 0.01451 1.06000

D17 -3.13366 0.00065 0.05524 -0.04703 0.00829 -3.12537

D18 3.08701 -0.00110 0.07012 0.20545 0.27495 -2.92122

D19 -1.00150 0.00040 0.08235 0.19344 0.27624 -0.72526

D20 1.11097 -0.00013 0.07220 0.21583 0.28821 1.39919

D21 1.84728 0.00019 -0.00635 0.00854 0.00215 1.84943

D22 -1.05967 -0.00180 -0.05121 -0.09409 -0.14527 -1.20494

D23 2.52764 -0.00059 0.03468 -0.03301 0.00139 2.52903

D24 -0.84856 0.00092 0.07801 0.06988 0.14817 -0.70038

D25 3.04184 0.00053 0.20093 -0.05335 0.14752 -3.09382

D26 -1.12562 0.00059 0.20292 -0.04055 0.16232 -0.96330

D27 0.92218 -0.00017 0.19248 -0.04858 0.14401 1.06619

D28 3.11317 0.00058 0.05715 0.01651 0.07370 -3.09632

D29 -1.04118 0.00028 0.04938 0.01358 0.06302 -0.97817

D30 0.99129 0.00060 0.05496 0.01196 0.06697 1.05827

D31 1.03444 -0.00035 0.05637 0.00676 0.06306 1.09750

D32 -3.11992 -0.00064 0.04860 0.00383 0.05238 -3.06753

D33 -1.08744 -0.00032 0.05417 0.00220 0.05634 -1.03110

D34 -1.07644 0.00020 0.06541 0.00737 0.07276 -1.00367

D35 1.05240 -0.00010 0.05764 0.00444 0.06208 1.11448

D36 3.08487 0.00023 0.06321 0.00281 0.06604 -3.13228

D37 -3.06975 -0.00081 -0.06209 -0.05334 -0.11545 3.09799

D38 -0.94980 -0.00033 -0.05139 -0.04495 -0.09632 -1.04612

D39 1.07786 -0.00059 -0.05713 -0.05077 -0.10790 0.96996

D40 1.08257 -0.00026 -0.05825 -0.04857 -0.10684 0.97573

D41 -3.08066 0.00021 -0.04755 -0.04018 -0.08771 3.11481

D42 -1.05301 -0.00005 -0.05329 -0.04600 -0.09929 -1.15230

D43 -0.94299 -0.00037 -0.06137 -0.04520 -0.10659 -1.04957

D44 1.17696 0.00011 -0.05067 -0.03681 -0.08746 1.08950

D45 -3.07857 -0.00015 -0.05641 -0.04262 -0.09903 3.10558

D46 3.12205 0.00044 0.01805 0.01844 0.03651 -3.12463

D47 -1.06446 0.00041 0.01616 0.02043 0.03661 -1.02785

D48 1.02745 0.00036 0.01665 0.02014 0.03681 1.06426

D49 1.00472 -0.00010 0.00825 0.00920 0.01743 1.02215

D50 3.10139 -0.00013 0.00636 0.01118 0.01753 3.11892

D51 -1.08988 -0.00018 0.00685 0.01090 0.01773 -1.07215

D52 -1.02602 -0.00007 0.01075 0.01417 0.02493 -1.00109

D53 1.07065 -0.00010 0.00887 0.01616 0.02503 1.09568

D54 -3.12062 -0.00015 0.00936 0.01587 0.02523 -3.09539

Item Value Threshold Converged?

Maximum Force 0.003160 0.000450 NO

RMS Force 0.000922 0.000300 NO

Maximum Displacement 1.321785 0.001800 NO

RMS Displacement 0.276541 0.001200 NO

Predicted change in Energy=-6.957441D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:42:30 2019, MaxMem= 1342177280 cpu: 0.6

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.032504 -0.502567 -0.289379

2 6 0 -2.903065 0.113263 0.488662

3 8 0 -4.641509 0.062406 -1.160958

4 8 0 -4.298093 -1.777915 0.070515

5 6 0 -2.354910 -0.685010 1.650037

6 16 0 -1.575610 0.389792 -0.876227

7 6 0 -0.107588 0.757423 -0.006673

8 16 0 1.081795 -0.578762 0.003996

9 16 0 0.110079 2.222668 0.871590

10 6 0 2.692488 0.308388 -0.064404

11 6 0 3.852404 -0.675375 -0.131775

12 6 0 5.204668 0.042108 -0.125055

13 6 0 6.385769 -0.923173 -0.130614

14 1 0 -3.232354 1.099565 0.810790

15 1 0 -5.003990 -2.099228 -0.512145

16 1 0 -1.523838 -0.151475 2.107535

17 1 0 -3.126692 -0.826205 2.410770

18 1 0 -2.005553 -1.669908 1.341533

19 1 0 2.670571 0.960109 -0.938901

20 1 0 2.767138 0.936422 0.822105

21 1 0 3.803264 -1.363422 0.719794

22 1 0 3.771468 -1.294417 -1.031696

23 1 0 5.268314 0.710904 -0.990805

24 1 0 5.263181 0.687256 0.758462

25 1 0 7.341306 -0.391960 -0.108450

26 1 0 6.360575 -1.589469 0.736899

27 1 0 6.384845 -1.553054 -1.025384

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.503405 0.000000

3 O 1.204047 2.397085 0.000000

4 O 1.351508 2.386944 2.240813 0.000000

5 C 2.570786 1.512119 3.699845 2.732268 0.000000

6 S 2.678997 1.923935 3.096448 3.606548 2.853859

7 C 4.131885 2.911184 4.729891 4.898391 3.142572

8 S 5.123273 4.073439 5.875749 5.512312 3.812044

9 S 5.092716 3.698008 5.601391 6.006527 3.890597

10 C 6.777447 5.626204 7.419600 7.296512 5.422396

11 C 7.888377 6.829587 8.587788 8.227218 6.457995

12 C 9.254676 8.131239 9.900541 9.677458 7.799158

13 C 10.427969 9.366971 11.119075 10.719885 8.923391

14 H 2.101771 1.088573 2.636135 3.156533 2.158460

15 H 1.882216 3.211015 2.285828 0.970065 3.700360

16 H 3.487387 2.143153 4.522020 3.806737 1.088414

17 H 2.866364 2.151072 3.980143 2.784730 1.092840

18 H 2.851507 2.170856 4.026367 2.623526 1.089610

19 H 6.891482 5.815540 7.370326 7.554997 5.887655

20 H 7.038552 5.739336 7.719099 7.605918 5.435980

21 H 7.947249 6.870871 8.768375 8.137895 6.264878

22 H 7.879089 6.988737 8.522668 8.158827 6.715324

23 H 9.405835 8.325709 9.932476 9.941667 8.187561

24 H 9.429921 8.190839 10.108289 9.897893 7.791876

25 H 11.375787 10.274187 12.037528 11.722990 9.858740

26 H 10.500033 9.422098 11.286115 10.681141 8.809741

27 H 10.496018 9.556893 11.144890 10.741355 9.181214

6 7 8 9 10

6 S 0.000000

7 C 1.745384 0.000000

8 S 2.962210 1.788893 0.000000

9 S 3.042343 1.722111 3.089493 0.000000

10 C 4.345382 2.836440 1.840122 3.348043 0.000000

11 C 5.581409 4.213087 2.775616 4.838429 1.522410

12 C 6.830616 5.361506 4.171357 5.630540 2.526980

13 C 8.103294 6.708461 5.316849 7.091193 3.893770

14 H 2.468725 3.247994 4.698891 3.526601 6.041165

15 H 4.252242 5.691284 6.294044 6.837194 8.076686

16 H 3.032900 2.702172 3.375910 3.135889 4.765102

17 H 3.832604 4.179342 4.854395 4.705464 6.424691

18 H 3.057069 3.363312 3.537134 4.455210 5.287901

19 H 4.284769 2.937397 2.404453 3.380541 1.090856

20 H 4.694954 2.997159 2.409454 2.952429 1.088990

21 H 5.878207 4.507826 2.921378 5.150019 2.154933

22 H 5.608206 4.506417 2.969708 5.422007 2.160749

23 H 6.852410 5.465436 4.492194 5.688702 2.766787

24 H 7.037738 5.425451 4.433510 5.378173 2.725639

25 H 8.983986 7.537736 6.263307 7.751606 4.701482

26 H 8.336826 6.920833 5.424407 7.322515 4.206995

27 H 8.195470 6.966187 5.489190 7.564871 4.245226

11 12 13 14 15

11 C 0.000000

12 C 1.530831 0.000000

13 C 2.545455 1.525385 0.000000

14 H 7.364281 8.554376 9.873500 0.000000

15 H 8.978182 10.438000 11.456670 3.888590 0.000000

16 H 5.847474 7.091877 8.256313 2.483078 4.771574

17 H 7.429339 8.751910 9.846571 2.505931 3.699766

18 H 6.121715 7.554413 8.552141 3.075176 3.551206

19 H 2.173245 2.815443 4.242968 6.158359 8.272881

20 H 2.164621 2.763777 4.178548 6.001720 8.449013

21 H 1.095898 2.157132 2.754333 7.454830 8.923385

22 H 1.095273 2.159250 2.790043 7.627544 8.827588

23 H 2.159745 1.095838 2.158435 8.698169 10.660496

24 H 2.153967 1.095555 2.155027 8.505695 10.714184

25 H 3.500472 2.180347 1.093494 10.717832 12.469325

26 H 2.807326 2.177413 1.094150 9.962963 11.444356

27 H 2.825263 2.178980 1.094241 10.143886 11.413469

16 17 18 19 20

16 H 0.000000

17 H 1.765320 0.000000

18 H 1.767610 1.764103 0.000000

19 H 5.301835 6.929609 5.829537 0.000000

20 H 4.609590 6.353577 5.462722 1.763811 0.000000

21 H 5.636723 7.153481 5.850029 3.071329 2.524541

22 H 6.261098 7.723627 6.256771 2.510672 3.069512

23 H 7.515100 9.187466 8.001074 2.610184 3.097318

24 H 6.970444 8.683931 7.663595 3.110806 2.509256

25 H 9.141072 10.775622 9.544599 4.932900 4.853200

26 H 8.130832 9.663988 8.388334 4.787983 4.393197

27 H 8.621303 10.139270 8.718642 4.485454 4.764296

21 22 23 24 25

21 H 0.000000

22 H 1.753138 0.000000

23 H 3.061919 2.502704 0.000000

24 H 2.517565 3.058905 1.749434 0.000000

25 H 3.761312 3.796124 2.508417 2.496967 0.000000

26 H 2.567339 3.149358 3.077289 2.527492 1.763654

27 H 3.121885 2.626151 2.524548 3.075585 1.761739

26 27

26 H 0.000000

27 H 1.762826 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 8.06D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.066414 -0.544454 -0.192172

2 6 0 -2.927298 0.210910 0.433981

3 8 0 -4.675883 -0.170173 -1.160775

4 8 0 -4.340428 -1.712770 0.429541

5 6 0 -2.378889 -0.329778 1.735291

6 16 0 -1.605734 0.181146 -0.963913

7 6 0 -0.129568 0.710013 -0.197362

8 16 0 1.048731 -0.604991 0.089886

9 16 0 0.105465 2.325335 0.351419

10 6 0 2.666294 0.232699 -0.170524

11 6 0 3.817588 -0.753983 -0.033728

12 6 0 5.175773 -0.063890 -0.183892

13 6 0 6.348772 -1.019680 0.009344

14 1 0 -3.246472 1.245987 0.542306

15 1 0 -5.052419 -2.143036 -0.069425

16 1 0 -1.540713 0.280384 2.066666

17 1 0 -3.147279 -0.300250 2.511825

18 1 0 -2.039554 -1.360799 1.639906

19 1 0 2.644585 0.685666 -1.162651

20 1 0 2.751420 1.032728 0.563374

21 1 0 3.767805 -1.246624 0.943932

22 1 0 3.726169 -1.547990 -0.782607

23 1 0 5.239815 0.406808 -1.171416

24 1 0 5.244888 0.752387 0.543539

25 1 0 7.308797 -0.504695 -0.084847

26 1 0 6.323209 -1.487922 0.997907

27 1 0 6.337302 -1.823944 -0.732540

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2544566 0.1940153 0.1823738

Leave Link 202 at Sat Aug 17 17:42:30 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.5271175032 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0548183269 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.4722991762 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2314

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.20D-08

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 104

GePol: Fraction of low-weight points (<1% of avg) = 4.49%

GePol: Cavity surface area = 308.423 Ang\*\*2

GePol: Cavity volume = 319.487 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0056483951 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.4666507812 Hartrees.

Leave Link 301 at Sat Aug 17 17:42:30 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.83D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:42:30 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:42:30 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999345 0.035940 0.001711 0.003893 Ang= 4.15 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7553 S= 0.5027

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.63088126352

Leave Link 401 at Sat Aug 17 17:42:31 2019, MaxMem= 1342177280 cpu: 7.5

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16063788.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.33D-15 for 2313.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.82D-15 for 1443 1210.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.44D-15 for 2313.

Iteration 1 A^-1\*A deviation from orthogonality is 9.14D-12 for 969 967.

E= -1658.28944709123

DIIS: error= 2.58D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.28944709123 IErMin= 1 ErrMin= 2.58D-02

ErrMax= 2.58D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.99D-01 BMatP= 8.99D-01

IDIUse=3 WtCom= 7.42D-01 WtEn= 2.58D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Recover alternate guess density for next cycle.

RMSDP=2.92D-03 MaxDP=8.26D-02 OVMax= 0.00D+00

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.91D-03 CP: 9.86D-01

E= -1658.21883613379 Delta-E= 0.070610957448 Rises=F Damp=F

Switch densities from cycles 1 and 2 for lowest energy.

DIIS: error= 5.07D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 1 EnMin= -1658.28944709123 IErMin= 1 ErrMin= 2.58D-02

ErrMax= 5.07D-02 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.20D+00 BMatP= 8.99D-01

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.728D+00 0.272D+00

Coeff: 0.728D+00 0.272D+00

Gap= 0.114 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=1.39D-02 MaxDP=5.42D-01 DE= 7.06D-02 OVMax= 1.88D-01

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.96D-03 CP: 9.87D-01 3.53D-01

E= -1658.59242925484 Delta-E= -0.373593121054 Rises=F Damp=F

DIIS: error= 2.29D-02 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.59242925484 IErMin= 3 ErrMin= 2.29D-02

ErrMax= 2.29D-02 0.00D+00 EMaxC= 1.00D+00 BMatC= 4.13D-01 BMatP= 8.99D-01

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.558D-01 0.271D+00 0.673D+00

Coeff: 0.558D-01 0.271D+00 0.673D+00

Gap= 0.127 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=9.43D-04 MaxDP=5.71D-02 DE=-3.74D-01 OVMax= 6.24D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 5.61D-04 CP: 9.85D-01 5.12D-01 6.94D-01

E= -1658.66266651711 Delta-E= -0.070237262270 Rises=F Damp=F

DIIS: error= 8.85D-03 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.66266651711 IErMin= 4 ErrMin= 8.85D-03

ErrMax= 8.85D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 6.89D-02 BMatP= 4.13D-01

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.191D-01 0.121D+00 0.384D+00 0.514D+00

Coeff: -0.191D-01 0.121D+00 0.384D+00 0.514D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.130 Goal= None Shift= 0.000

RMSDP=3.61D-04 MaxDP=1.95D-02 DE=-7.02D-02 OVMax= 3.80D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.23D-04 CP: 9.86D-01 5.25D-01 7.31D-01 5.16D-01

E= -1658.67373728923 Delta-E= -0.011070772123 Rises=F Damp=F

DIIS: error= 3.50D-03 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67373728923 IErMin= 5 ErrMin= 3.50D-03

ErrMax= 3.50D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 8.91D-03 BMatP= 6.89D-02

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.103D-01 0.231D-01 0.118D+00 0.301D+00 0.569D+00

Coeff: -0.103D-01 0.231D-01 0.118D+00 0.301D+00 0.569D+00

Gap= 0.124 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=1.49D-04 MaxDP=6.25D-03 DE=-1.11D-02 OVMax= 1.48D-02

Cycle 6 Pass 1 IDiag 1:

RMSU= 9.16D-05 CP: 9.86D-01 5.19D-01 7.36D-01 6.31D-01 5.74D-01

E= -1658.67543286097 Delta-E= -0.001695571742 Rises=F Damp=F

DIIS: error= 1.62D-03 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67543286097 IErMin= 6 ErrMin= 1.62D-03

ErrMax= 1.62D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.13D-03 BMatP= 8.91D-03

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.318D-02 0.328D-02 0.392D-01 0.139D+00 0.346D+00 0.475D+00

Coeff: -0.318D-02 0.328D-02 0.392D-01 0.139D+00 0.346D+00 0.475D+00

Gap= 0.125 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=4.16D-05 MaxDP=1.92D-03 DE=-1.70D-03 OVMax= 4.44D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.93D-05 CP: 9.86D-01 5.16D-01 7.39D-01 6.41D-01 6.57D-01

CP: 7.95D-01

E= -1658.67564251563 Delta-E= -0.000209654659 Rises=F Damp=F

DIIS: error= 2.49D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67564251563 IErMin= 7 ErrMin= 2.49D-04

ErrMax= 2.49D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 5.13D-05 BMatP= 1.13D-03

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.708D-03-0.680D-03 0.544D-02 0.335D-01 0.103D+00 0.216D+00

Coeff-Com: 0.643D+00

Coeff: -0.708D-03-0.680D-03 0.544D-02 0.335D-01 0.103D+00 0.216D+00

Coeff: 0.643D+00

Gap= 0.126 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=1.58D-05 MaxDP=5.42D-04 DE=-2.10D-04 OVMax= 1.91D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.25D-05 CP: 9.86D-01 5.15D-01 7.39D-01 6.50D-01 6.87D-01

CP: 8.35D-01 8.95D-01

E= -1658.67565439335 Delta-E= -0.000011877713 Rises=F Damp=F

DIIS: error= 9.30D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67565439335 IErMin= 8 ErrMin= 9.30D-05

ErrMax= 9.30D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 8.11D-06 BMatP= 5.13D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.172D-04-0.799D-03-0.211D-02 0.402D-03 0.123D-01 0.519D-01

Coeff-Com: 0.306D+00 0.632D+00

Coeff: 0.172D-04-0.799D-03-0.211D-02 0.402D-03 0.123D-01 0.519D-01

Coeff: 0.306D+00 0.632D+00

Gap= 0.126 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=8.88D-06 MaxDP=3.27D-04 DE=-1.19D-05 OVMax= 1.37D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 4.81D-06 CP: 9.86D-01 5.15D-01 7.38D-01 6.55D-01 6.91D-01

CP: 8.92D-01 1.04D+00 1.06D+00

E= -1658.67565717802 Delta-E= -0.000002784678 Rises=F Damp=F

DIIS: error= 2.84D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67565717802 IErMin= 9 ErrMin= 2.84D-05

ErrMax= 2.84D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.22D-06 BMatP= 8.11D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.178D-03-0.139D-03-0.203D-02-0.757D-02-0.180D-01-0.293D-01

Coeff-Com: -0.499D-01 0.196D+00 0.910D+00

Coeff: 0.178D-03-0.139D-03-0.203D-02-0.757D-02-0.180D-01-0.293D-01

Coeff: -0.499D-01 0.196D+00 0.910D+00

Gap= 0.126 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=5.59D-06 MaxDP=2.39D-04 DE=-2.78D-06 OVMax= 7.97D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 2.20D-06 CP: 9.86D-01 5.15D-01 7.38D-01 6.57D-01 6.98D-01

CP: 9.25D-01 1.12D+00 1.29D+00 1.03D+00

E= -1658.67565791829 Delta-E= -0.000000740260 Rises=F Damp=F

DIIS: error= 1.50D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67565791829 IErMin=10 ErrMin= 1.50D-05

ErrMax= 1.50D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 5.57D-07 BMatP= 1.22D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.105D-03 0.103D-03-0.810D-03-0.486D-02-0.138D-01-0.288D-01

Coeff-Com: -0.926D-01-0.130D-01 0.548D+00 0.605D+00

Coeff: 0.105D-03 0.103D-03-0.810D-03-0.486D-02-0.138D-01-0.288D-01

Coeff: -0.926D-01-0.130D-01 0.548D+00 0.605D+00

Gap= 0.126 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=3.27D-06 MaxDP=1.45D-04 DE=-7.40D-07 OVMax= 5.71D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.10D-06 CP: 9.86D-01 5.15D-01 7.38D-01 6.59D-01 7.01D-01

CP: 9.41D-01 1.16D+00 1.40D+00 1.34D+00 7.87D-01

E= -1658.67565810271 Delta-E= -0.000000184421 Rises=F Damp=F

DIIS: error= 8.39D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67565810271 IErMin=11 ErrMin= 8.39D-06

ErrMax= 8.39D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.02D-07 BMatP= 5.57D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.399D-04 0.697D-04-0.144D-03-0.159D-02-0.489D-02-0.115D-01

Coeff-Com: -0.432D-01-0.390D-01 0.164D+00 0.350D+00 0.586D+00

Coeff: 0.399D-04 0.697D-04-0.144D-03-0.159D-02-0.489D-02-0.115D-01

Coeff: -0.432D-01-0.390D-01 0.164D+00 0.350D+00 0.586D+00

Gap= 0.126 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=7.87D-07 MaxDP=5.88D-05 DE=-1.84D-07 OVMax= 1.47D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 5.06D-07 CP: 9.86D-01 5.15D-01 7.38D-01 6.59D-01 7.01D-01

CP: 9.41D-01 1.16D+00 1.42D+00 1.35D+00 9.49D-01

CP: 6.90D-01

E= -1658.67565813395 Delta-E= -0.000000031248 Rises=F Damp=F

DIIS: error= 3.06D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.67565813395 IErMin=12 ErrMin= 3.06D-06

ErrMax= 3.06D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.89D-08 BMatP= 1.02D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.514D-05 0.150D-04 0.125D-03 0.286D-03 0.613D-03 0.446D-03

Coeff-Com: -0.202D-02-0.173D-01-0.415D-01 0.333D-01 0.336D+00 0.690D+00

Coeff: -0.514D-05 0.150D-04 0.125D-03 0.286D-03 0.613D-03 0.446D-03

Coeff: -0.202D-02-0.173D-01-0.415D-01 0.333D-01 0.336D+00 0.690D+00

Gap= 0.126 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=4.31D-07 MaxDP=2.23D-05 DE=-3.12D-08 OVMax= 4.32D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.95D-07 CP: 9.86D-01 5.15D-01 7.38D-01 6.59D-01 7.02D-01

CP: 9.43D-01 1.16D+00 1.43D+00 1.39D+00 1.00D+00

CP: 8.83D-01 8.59D-01

E= -1658.67565814016 Delta-E= -0.000000006206 Rises=F Damp=F

DIIS: error= 1.12D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1658.67565814016 IErMin=13 ErrMin= 1.12D-06

ErrMax= 1.12D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.33D-09 BMatP= 1.89D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.708D-05-0.335D-05 0.716D-04 0.342D-03 0.905D-03 0.170D-02

Coeff-Com: 0.475D-02-0.136D-02-0.364D-01-0.343D-01 0.729D-01 0.277D+00

Coeff-Com: 0.714D+00

Coeff: -0.708D-05-0.335D-05 0.716D-04 0.342D-03 0.905D-03 0.170D-02

Coeff: 0.475D-02-0.136D-02-0.364D-01-0.343D-01 0.729D-01 0.277D+00

Coeff: 0.714D+00

Gap= 0.126 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=1.17D-07 MaxDP=7.18D-06 DE=-6.21D-09 OVMax= 2.39D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 6.47D-08 CP: 9.86D-01 5.15D-01 7.38D-01 6.59D-01 7.01D-01

CP: 9.43D-01 1.16D+00 1.43D+00 1.39D+00 1.01D+00

CP: 9.31D-01 9.94D-01 9.02D-01

E= -1658.67565814066 Delta-E= -0.000000000495 Rises=F Damp=F

DIIS: error= 3.17D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1658.67565814066 IErMin=14 ErrMin= 3.17D-07

ErrMax= 3.17D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.01D-10 BMatP= 1.33D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.198D-05-0.274D-05 0.952D-05 0.889D-04 0.245D-03 0.584D-03

Coeff-Com: 0.216D-02 0.191D-02-0.892D-02-0.196D-01-0.133D-01 0.125D-01

Coeff-Com: 0.279D+00 0.746D+00

Coeff: -0.198D-05-0.274D-05 0.952D-05 0.889D-04 0.245D-03 0.584D-03

Coeff: 0.216D-02 0.191D-02-0.892D-02-0.196D-01-0.133D-01 0.125D-01

Coeff: 0.279D+00 0.746D+00

Gap= 0.126 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=5.23D-08 MaxDP=3.77D-06 DE=-4.95D-10 OVMax= 5.33D-06

Cycle 15 Pass 1 IDiag 1:

RMSU= 2.76D-08 CP: 9.86D-01 5.15D-01 7.38D-01 6.59D-01 7.01D-01

CP: 9.43D-01 1.16D+00 1.43D+00 1.39D+00 1.02D+00

CP: 9.45D-01 1.03D+00 1.06D+00 9.16D-01

E= -1658.67565814075 Delta-E= -0.000000000093 Rises=F Damp=F

DIIS: error= 1.13D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1658.67565814075 IErMin=15 ErrMin= 1.13D-07

ErrMax= 1.13D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 4.09D-11 BMatP= 2.01D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.387D-06-0.438D-06-0.985D-05-0.267D-04-0.703D-04-0.825D-04

Coeff-Com: -0.892D-04 0.921D-03 0.383D-02-0.136D-02-0.178D-01-0.529D-01

Coeff-Com: -0.174D-01 0.351D+00 0.734D+00

Coeff: 0.387D-06-0.438D-06-0.985D-05-0.267D-04-0.703D-04-0.825D-04

Coeff: -0.892D-04 0.921D-03 0.383D-02-0.136D-02-0.178D-01-0.529D-01

Coeff: -0.174D-01 0.351D+00 0.734D+00

Gap= 0.126 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=2.15D-08 MaxDP=1.63D-06 DE=-9.32D-11 OVMax= 4.99D-06

Cycle 16 Pass 1 IDiag 1:

RMSU= 9.45D-09 CP: 9.86D-01 5.15D-01 7.38D-01 6.59D-01 7.01D-01

CP: 9.43D-01 1.16D+00 1.43D+00 1.39D+00 1.02D+00

CP: 9.51D-01 1.04D+00 1.10D+00 1.10D+00 8.44D-01

E= -1658.67565814074 Delta-E= 0.000000000005 Rises=F Damp=F

DIIS: error= 3.14D-08 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=15 EnMin= -1658.67565814075 IErMin=16 ErrMin= 3.14D-08

ErrMax= 3.14D-08 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.18D-12 BMatP= 4.09D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.335D-06 0.357D-07-0.403D-05-0.163D-04-0.435D-04-0.757D-04

Coeff-Com: -0.222D-03 0.859D-04 0.208D-02 0.127D-02-0.435D-02-0.200D-01

Coeff-Com: -0.320D-01 0.443D-01 0.267D+00 0.742D+00

Coeff: 0.335D-06 0.357D-07-0.403D-05-0.163D-04-0.435D-04-0.757D-04

Coeff: -0.222D-03 0.859D-04 0.208D-02 0.127D-02-0.435D-02-0.200D-01

Coeff: -0.320D-01 0.443D-01 0.267D+00 0.742D+00

Gap= 0.126 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=6.32D-09 MaxDP=3.69D-07 DE= 5.00D-12 OVMax= 6.37D-07

Error on total polarization charges = 0.04183

SCF Done: E(UB3LYP) = -1658.67565814 A.U. after 16 cycles

NFock= 16 Conv=0.63D-08 -V/T= 2.0020

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655287818716D+03 PE=-6.147798681145D+03 EE= 1.731368553507D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.54

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:43:03 2019, MaxMem= 1342177280 cpu: 381.6

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 334

Leave Link 701 at Sat Aug 17 17:43:04 2019, MaxMem= 1342177280 cpu: 10.2

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:43:04 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:43:07 2019, MaxMem= 1342177280 cpu: 36.0

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.16562956D+00-2.85879687D+00 7.52164980D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.005247665 -0.003819325 0.012036285

2 6 0.001187920 -0.002198356 -0.003403350

3 8 -0.006682515 0.004340498 -0.008845188

4 8 0.001882579 0.000144962 -0.000688831

5 6 -0.001294993 -0.001183627 0.000237747

6 16 -0.001307987 -0.000368403 -0.000101636

7 6 0.000370026 0.002237164 -0.000146843

8 16 0.000484743 -0.001339959 0.000449104

9 16 -0.000260617 0.000453186 0.001525395

10 6 -0.001476129 -0.000071562 0.000609945

11 6 -0.000015092 -0.000792680 -0.000422373

12 6 -0.000143363 0.000635199 0.000558270

13 6 0.001064316 -0.000990051 -0.000463588

14 1 0.001382573 0.001995798 -0.000803192

15 1 -0.001856897 -0.000937600 -0.000919579

16 1 0.001320988 0.000764267 0.000451889

17 1 -0.000569384 0.000323372 0.000850136

18 1 0.000547886 -0.000384649 -0.000631879

19 1 0.000496238 0.000484396 -0.000878376

20 1 0.000106943 0.000333100 0.000503967

21 1 0.000165481 0.000060703 0.000648709

22 1 -0.000200228 -0.000021522 -0.000702265

23 1 -0.000095525 -0.000149466 -0.000605083

24 1 0.000126652 0.000085908 0.000712618

25 1 0.000235140 0.000607878 0.000056166

26 1 -0.000266181 -0.000072816 0.000577040

27 1 -0.000450239 -0.000136416 -0.000605089

-------------------------------------------------------------------

Cartesian Forces: Max 0.012036285 RMS 0.002203318

Leave Link 716 at Sat Aug 17 17:43:07 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.011809038 RMS 0.001457193

Search for a local minimum.

Step number 29 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .14572D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 29 27

DE= 1.32D-03 DEPred=-6.96D-04 R=-1.89D+00

Trust test=-1.89D+00 RLast= 1.00D+00 DXMaxT set to 5.00D-02

ITU= -1 -1 0 0 -1 0 0 -1 1 -1 1 -1 1 1 -1 1 -1 1 1 -1

ITU= 0 0 -1 0 0 -1 -1 0 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.95385.

Iteration 1 RMS(Cart)= 0.12349619 RMS(Int)= 0.03265481

Iteration 2 RMS(Cart)= 0.05007439 RMS(Int)= 0.00224127

Iteration 3 RMS(Cart)= 0.00280866 RMS(Int)= 0.00001139

Iteration 4 RMS(Cart)= 0.00000829 RMS(Int)= 0.00000998

Iteration 5 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000998

ITry= 1 IFail=0 DXMaxC= 6.76D-01 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=T

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.84102 0.00035 -0.00356 0.00000 -0.00356 2.83747

R2 2.27532 0.01181 0.01188 0.00000 0.01188 2.28720

R3 2.55398 0.00036 -0.00091 0.00000 -0.00091 2.55307

R4 2.85749 0.00092 0.00869 0.00000 0.00869 2.86618

R5 3.63571 -0.00184 -0.03704 0.00000 -0.03704 3.59867

R6 2.05710 0.00115 0.00081 0.00000 0.00081 2.05792

R7 1.83316 0.00220 0.00352 0.00000 0.00352 1.83667

R8 2.05680 0.00159 0.00434 0.00000 0.00434 2.06115

R9 2.06517 0.00095 0.00335 0.00000 0.00335 2.06852

R10 2.05906 0.00068 0.00112 0.00000 0.00112 2.06019

R11 3.29830 0.00127 0.02097 0.00000 0.02097 3.31927

R12 3.38052 0.00107 0.00344 0.00000 0.00344 3.38396

R13 3.25432 0.00112 -0.00031 0.00000 -0.00031 3.25401

R14 3.47733 -0.00042 -0.00112 0.00000 -0.00112 3.47621

R15 2.87694 0.00084 0.00378 0.00000 0.00378 2.88072

R16 2.06142 0.00099 0.00213 0.00000 0.00213 2.06355

R17 2.05789 0.00060 0.00218 0.00000 0.00218 2.06007

R18 2.89285 0.00041 0.00130 0.00000 0.00130 2.89416

R19 2.07095 0.00047 0.00127 0.00000 0.00127 2.07222

R20 2.06977 0.00060 0.00103 0.00000 0.00103 2.07079

R21 2.88256 0.00083 0.00313 0.00000 0.00313 2.88569

R22 2.07083 0.00039 0.00106 0.00000 0.00106 2.07189

R23 2.07030 0.00063 0.00130 0.00000 0.00130 2.07160

R24 2.06640 0.00050 0.00115 0.00000 0.00115 2.06756

R25 2.06764 0.00052 0.00142 0.00000 0.00142 2.06906

R26 2.06782 0.00056 0.00109 0.00000 0.00109 2.06890

A1 2.16808 0.00154 0.00884 0.00000 0.00884 2.17692

A2 1.97835 0.00022 -0.00249 0.00000 -0.00249 1.97586

A3 2.13667 -0.00177 -0.00680 0.00000 -0.00680 2.12987

A4 2.04156 -0.00192 -0.01741 0.00000 -0.01740 2.02416

A5 1.78245 0.00325 0.05280 0.00000 0.05279 1.83524

A6 1.87238 0.00052 -0.00079 0.00000 -0.00080 1.87158

A7 1.95048 -0.00115 -0.00398 0.00000 -0.00397 1.94651

A8 1.93981 0.00085 0.00025 0.00000 0.00027 1.94008

A9 1.86337 -0.00141 -0.02992 0.00000 -0.02991 1.83346

A10 1.87090 0.00074 0.00214 0.00000 0.00214 1.87304

A11 1.91862 -0.00025 -0.00671 0.00000 -0.00670 1.91191

A12 1.92499 0.00012 0.00351 0.00000 0.00351 1.92850

A13 1.95622 -0.00043 -0.00374 0.00000 -0.00374 1.95248

A14 1.88596 0.00001 -0.00214 0.00000 -0.00214 1.88383

A15 1.89366 0.00009 -0.00034 0.00000 -0.00034 1.89332

A16 1.88256 0.00048 0.00959 0.00000 0.00959 1.89215

A17 1.83088 -0.00582 -0.03623 0.00000 -0.03623 1.79465

A18 1.98762 -0.00265 -0.01509 0.00000 -0.01503 1.97259

A19 2.14076 0.00133 0.00118 0.00000 0.00125 2.14201

A20 2.15130 0.00108 0.00278 0.00000 0.00284 2.15414

A21 1.79430 0.00201 -0.00114 0.00000 -0.00114 1.79316

A22 1.93586 -0.00166 -0.00699 0.00000 -0.00699 1.92887

A23 1.87575 0.00083 -0.00106 0.00000 -0.00106 1.87469

A24 1.88366 0.00066 0.01091 0.00000 0.01091 1.89457

A25 1.94539 -0.00033 -0.00641 0.00000 -0.00641 1.93897

A26 1.93528 0.00059 0.00298 0.00000 0.00298 1.93826

A27 1.88539 -0.00002 0.00108 0.00000 0.00108 1.88647

A28 1.94977 0.00080 0.00252 0.00000 0.00252 1.95228

A29 1.91469 -0.00010 0.00312 0.00000 0.00312 1.91780

A30 1.92333 -0.00051 -0.00763 0.00000 -0.00763 1.91570

A31 1.90759 -0.00036 -0.00149 0.00000 -0.00149 1.90609

A32 1.91111 -0.00021 -0.00086 0.00000 -0.00086 1.91025

A33 1.85490 0.00035 0.00445 0.00000 0.00445 1.85935

A34 1.96857 -0.00010 -0.00124 0.00000 -0.00124 1.96734

A35 1.91121 -0.00018 -0.00452 0.00000 -0.00452 1.90669

A36 1.90363 0.00016 0.00304 0.00000 0.00304 1.90667

A37 1.91597 -0.00009 -0.00297 0.00000 -0.00297 1.91300

A38 1.91159 0.00002 0.00105 0.00000 0.00105 1.91264

A39 1.84900 0.00021 0.00504 0.00000 0.00504 1.85404

A40 1.94886 -0.00040 -0.00343 0.00000 -0.00343 1.94543

A41 1.94404 -0.00035 -0.00162 0.00000 -0.00162 1.94242

A42 1.94614 -0.00049 -0.00233 0.00000 -0.00233 1.94381

A43 1.87536 0.00037 0.00103 0.00000 0.00103 1.87639

A44 1.87230 0.00050 0.00446 0.00000 0.00446 1.87676

A45 1.87316 0.00047 0.00241 0.00000 0.00241 1.87557

D1 3.02537 -0.00002 -0.34226 0.00000 -0.34226 2.68311

D2 -1.12285 -0.00018 -0.31831 0.00000 -0.31830 -1.44115

D3 0.83319 -0.00018 -0.32921 0.00000 -0.32922 0.50397

D4 -0.13088 -0.00073 -0.36249 0.00000 -0.36249 -0.49337

D5 2.00408 -0.00089 -0.33854 0.00000 -0.33853 1.66555

D6 -2.32306 -0.00089 -0.34944 0.00000 -0.34945 -2.67251

D7 -3.09293 0.00000 -0.00977 0.00000 -0.00976 -3.10269

D8 0.03430 -0.00067 -0.02922 0.00000 -0.02923 0.00508

D9 3.10717 0.00057 0.05422 0.00000 0.05423 -3.12179

D10 -1.09815 0.00050 0.04957 0.00000 0.04958 -1.04857

D11 0.99967 0.00091 0.06166 0.00000 0.06166 1.06133

D12 1.06189 -0.00149 -0.00036 0.00000 -0.00036 1.06153

D13 3.13976 -0.00156 -0.00501 0.00000 -0.00501 3.13475

D14 -1.04561 -0.00115 0.00708 0.00000 0.00708 -1.03853

D15 -1.01787 0.00048 0.03964 0.00000 0.03964 -0.97823

D16 1.06000 0.00041 0.03499 0.00000 0.03499 1.09499

D17 -3.12537 0.00082 0.04707 0.00000 0.04707 -3.07830

D18 -2.92122 0.00094 -0.21525 0.00000 -0.21523 -3.13646

D19 -0.72526 0.00008 -0.20363 0.00000 -0.20363 -0.92889

D20 1.39919 -0.00048 -0.22457 0.00000 -0.22459 1.17459

D21 1.84943 -0.00169 -0.00282 0.00000 -0.00283 1.84660

D22 -1.20494 0.00125 0.08629 0.00000 0.08629 -1.11865

D23 2.52903 0.00109 0.02035 0.00000 0.02036 2.54938

D24 -0.70038 -0.00186 -0.06957 0.00000 -0.06958 -0.76996

D25 -3.09382 0.00053 0.09564 0.00000 0.09564 -2.99818

D26 -0.96330 -0.00035 0.08288 0.00000 0.08288 -0.88042

D27 1.06619 0.00040 0.08921 0.00000 0.08921 1.15540

D28 -3.09632 -0.00024 -0.00661 0.00000 -0.00661 -3.10293

D29 -0.97817 -0.00024 -0.00468 0.00000 -0.00468 -0.98284

D30 1.05827 -0.00017 -0.00191 0.00000 -0.00191 1.05636

D31 1.09750 0.00003 0.00352 0.00000 0.00353 1.10103

D32 -3.06753 0.00004 0.00546 0.00000 0.00546 -3.06208

D33 -1.03110 0.00011 0.00823 0.00000 0.00823 -1.02288

D34 -1.00367 -0.00012 0.00445 0.00000 0.00445 -0.99922

D35 1.11448 -0.00011 0.00638 0.00000 0.00638 1.12086

D36 -3.13228 -0.00004 0.00915 0.00000 0.00915 -3.12313

D37 3.09799 0.00035 0.05466 0.00000 0.05466 -3.13054

D38 -1.04612 0.00003 0.04676 0.00000 0.04676 -0.99936

D39 0.96996 0.00027 0.05198 0.00000 0.05198 1.02194

D40 0.97573 0.00020 0.05009 0.00000 0.05009 1.02582

D41 3.11481 -0.00012 0.04219 0.00000 0.04219 -3.12618

D42 -1.15230 0.00012 0.04741 0.00000 0.04741 -1.10489

D43 -1.04957 0.00010 0.04607 0.00000 0.04607 -1.00351

D44 1.08950 -0.00022 0.03817 0.00000 0.03817 1.12768

D45 3.10558 0.00002 0.04339 0.00000 0.04339 -3.13422

D46 -3.12463 -0.00018 -0.01378 0.00000 -0.01378 -3.13840

D47 -1.02785 -0.00024 -0.01591 0.00000 -0.01591 -1.04377

D48 1.06426 -0.00022 -0.01552 0.00000 -0.01552 1.04873

D49 1.02215 0.00019 -0.00499 0.00000 -0.00499 1.01716

D50 3.11892 0.00014 -0.00712 0.00000 -0.00712 3.11180

D51 -1.07215 0.00016 -0.00674 0.00000 -0.00674 -1.07889

D52 -1.00109 -0.00003 -0.00997 0.00000 -0.00997 -1.01106

D53 1.09568 -0.00008 -0.01210 0.00000 -0.01210 1.08358

D54 -3.09539 -0.00006 -0.01172 0.00000 -0.01172 -3.10711

Item Value Threshold Converged?

Maximum Force 0.011809 0.000450 NO

RMS Force 0.001457 0.000300 NO

Maximum Displacement 0.675597 0.001800 NO

RMS Displacement 0.141614 0.001200 NO

Predicted change in Energy=-1.795115D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:43:07 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.104029 -0.415292 -0.206146

2 6 0 -2.842542 0.062315 0.453485

3 8 0 -4.881224 0.294716 -0.803447

4 8 0 -4.282572 -1.750975 -0.109507

5 6 0 -2.345654 -0.771373 1.619028

6 16 0 -1.551976 0.148760 -0.944175

7 6 0 -0.109040 0.701450 -0.108894

8 16 0 1.104953 -0.594196 0.123865

9 16 0 -0.003230 2.246661 0.643588

10 6 0 2.698847 0.313543 -0.015361

11 6 0 3.869049 -0.662988 -0.044447

12 6 0 5.216181 0.063033 -0.105180

13 6 0 6.402358 -0.897578 -0.150675

14 1 0 -3.006118 1.096840 0.751693

15 1 0 -5.097857 -1.969486 -0.591383

16 1 0 -1.440742 -0.321756 2.029679

17 1 0 -3.096760 -0.804022 2.414610

18 1 0 -2.117589 -1.794246 1.318597

19 1 0 2.658501 0.906019 -0.931753

20 1 0 2.782090 0.999535 0.827784

21 1 0 3.843516 -1.302270 0.846133

22 1 0 3.774268 -1.329177 -0.909330

23 1 0 5.236234 0.714407 -0.986882

24 1 0 5.310685 0.722685 0.765268

25 1 0 7.353281 -0.357921 -0.190429

26 1 0 6.426136 -1.542153 0.734065

27 1 0 6.355392 -1.548169 -1.029962

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.501524 0.000000

3 O 1.210335 2.406265 0.000000

4 O 1.351024 2.382996 2.241604 0.000000

5 C 2.559285 1.516715 3.665249 2.774727 0.000000

6 S 2.715845 1.904333 3.335415 3.429550 2.836649

7 C 4.149278 2.863004 4.839584 4.840740 3.187061

8 S 5.222491 4.015267 6.122449 5.515254 3.764783

9 S 4.962317 3.587366 5.449662 5.904322 3.942963

10 C 6.844467 5.566859 7.620951 7.280887 5.412509

11 C 7.978564 6.769007 8.835188 8.224165 6.434394

12 C 9.333022 8.078064 10.124171 9.670416 7.800671

13 C 10.517597 9.314213 11.365161 10.719035 8.926112

14 H 2.099859 1.089003 2.564739 3.237446 2.163031

15 H 1.884574 3.210360 2.284406 0.971926 3.727736

16 H 3.478615 2.144048 4.499284 3.833378 1.090713

17 H 2.834443 2.158976 3.840238 2.945172 1.094612

18 H 2.858724 2.172739 4.062574 2.593936 1.090203

19 H 6.928506 5.735172 7.565554 7.477580 5.861885

20 H 7.105588 5.714452 7.866642 7.638931 5.482329

21 H 8.065823 6.835177 9.021783 8.194382 6.259796

22 H 7.962238 6.897513 8.807144 8.107423 6.645087

23 H 9.440672 8.232040 10.127820 9.871958 8.153731

24 H 9.532863 8.185866 10.320805 9.945592 7.847333

25 H 11.457465 10.224775 12.267226 11.719224 9.874938

26 H 10.631942 9.410708 11.558305 10.743912 8.849947

27 H 10.552800 9.454959 11.388989 10.679637 9.128459

6 7 8 9 10

6 S 0.000000

7 C 1.756482 0.000000

8 S 2.958372 1.790713 0.000000

9 S 3.052998 1.721947 3.093323 0.000000

10 C 4.354233 2.836097 1.839530 3.387089 0.000000

11 C 5.554814 4.206071 2.770070 4.892238 1.524412

12 C 6.820500 5.363354 4.169725 5.707113 2.531362

13 C 8.062003 6.704993 5.313182 7.179738 3.898861

14 H 2.426799 3.047951 4.489396 3.217314 5.809350

15 H 4.145443 5.679347 6.393579 6.727278 8.144483

16 H 3.012901 2.719168 3.191695 3.253376 4.660685

17 H 3.817798 4.190583 4.790191 4.691813 6.383006

18 H 3.035676 3.507206 3.640369 4.610323 5.424046

19 H 4.278051 2.894517 2.403848 3.371029 1.091984

20 H 4.758969 3.053662 2.418319 3.057329 1.090141

21 H 5.867030 4.533174 2.919378 5.237690 2.159466

22 H 5.527603 4.454685 2.955153 5.428412 2.157369

23 H 6.811870 5.416916 4.473665 5.697211 2.746430

24 H 7.095612 5.489811 4.453510 5.529467 2.756533

25 H 8.951450 7.537582 6.260687 7.848419 4.705876

26 H 8.326221 6.960808 5.439297 7.463246 4.230595

27 H 8.087855 6.906376 5.459715 7.591678 4.226785

11 12 13 14 15

11 C 0.000000

12 C 1.531521 0.000000

13 C 2.546364 1.527042 0.000000

14 H 7.141341 8.331217 9.659782 0.000000

15 H 9.078077 10.523635 11.558466 3.947351 0.000000

16 H 5.710720 7.001450 8.160866 2.469021 4.791604

17 H 7.388460 8.729611 9.839851 2.527209 3.794561

18 H 6.243194 7.698104 8.692081 3.077214 3.544112

19 H 2.171294 2.817015 4.228416 5.912555 8.279219

20 H 2.169389 2.769884 4.202708 5.789525 8.539478

21 H 1.096571 2.157141 2.775801 7.258246 9.080737

22 H 1.095816 2.159633 2.769240 7.390412 8.900881

23 H 2.157450 1.096398 2.158143 8.432393 10.684247

24 H 2.157322 1.096244 2.157765 8.325226 10.836329

25 H 3.500606 2.179832 1.094104 10.503383 12.561398

26 H 2.813842 2.178289 1.094900 9.794488 11.607835

27 H 2.817213 2.179219 1.094816 9.889805 11.469384

16 17 18 19 20

16 H 0.000000

17 H 1.767243 0.000000

18 H 1.769742 1.772163 0.000000

19 H 5.203970 6.873530 5.930139 0.000000

20 H 4.585048 6.350724 5.661533 1.766349 0.000000

21 H 5.503233 7.132727 6.000003 3.072732 2.534811

22 H 6.070338 7.650842 6.316164 2.498307 3.069997

23 H 7.399681 9.127680 8.104769 2.585432 3.065474

24 H 6.947759 8.702659 7.862593 3.153976 2.544474

25 H 9.070007 10.779080 9.697297 4.918136 4.875985

26 H 8.065714 9.698175 8.567407 4.792031 4.443876

27 H 8.464349 10.087715 8.795891 4.438433 4.765554

21 22 23 24 25

21 H 0.000000

22 H 1.757035 0.000000

23 H 3.060489 2.513880 0.000000

24 H 2.501912 3.061860 1.753750 0.000000

25 H 3.779511 3.777497 2.503220 2.500653 0.000000

26 H 2.596156 3.127060 3.077269 2.524815 1.765415

27 H 3.144793 2.593204 2.524603 3.077506 1.765584

26 27

26 H 0.000000

27 H 1.765455 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.31D-01

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.116268 -0.429740 -0.160014

2 6 0 -2.849119 0.117777 0.430860

3 8 0 -4.894225 0.207078 -0.833925

4 8 0 -4.299352 -1.743406 0.096950

5 6 0 -2.348606 -0.572483 1.685233

6 16 0 -1.566443 0.030328 -0.973981

7 6 0 -0.116533 0.672615 -0.218695

8 16 0 1.093836 -0.591259 0.161147

9 16 0 -0.000405 2.296362 0.342609

10 6 0 2.690348 0.286075 -0.094395

11 6 0 3.856615 -0.692163 -0.012514

12 6 0 5.206136 0.015280 -0.167030

13 6 0 6.388341 -0.949191 -0.103434

14 1 0 -3.006986 1.181305 0.603815

15 1 0 -5.118275 -2.014406 -0.350892

16 1 0 -1.439590 -0.080981 2.034189

17 1 0 -3.095158 -0.506193 2.483006

18 1 0 -2.126221 -1.625001 1.508329

19 1 0 2.646903 0.764661 -1.074955

20 1 0 2.781154 1.067765 0.660008

21 1 0 3.833853 -1.220014 0.948383

22 1 0 3.754220 -1.456746 -0.790808

23 1 0 5.223516 0.556223 -1.120533

24 1 0 5.308261 0.774040 0.617573

25 1 0 7.341073 -0.422471 -0.212667

26 1 0 6.414835 -1.483218 0.852035

27 1 0 6.333736 -1.700230 -0.898154

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3248118 0.1921106 0.1801260

Leave Link 202 at Sat Aug 17 17:43:07 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1101.6147400966 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0549283609 Hartrees.

Nuclear repulsion after empirical dispersion term = 1101.5598117357 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

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Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2317

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.12D-07

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 102

GePol: Fraction of low-weight points (<1% of avg) = 4.40%

GePol: Cavity surface area = 309.366 Ang\*\*2

GePol: Cavity volume = 320.177 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057950278 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1101.5540167079 Hartrees.

Leave Link 301 at Sat Aug 17 17:43:08 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:43:08 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:43:08 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Lowest energy guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000771 0.000016 0.000141 Ang= 0.09 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999609 -0.027784 -0.001205 -0.003047 Ang= -3.21 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 4.61D-02

Max alpha theta= 12.821 degrees.

Max beta theta= 13.054 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 17:43:08 2019, MaxMem= 1342177280 cpu: 4.2

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16105467.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.99D-15 for 2317.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.02D-15 for 1525 1174.

Iteration 1 A^-1\*A deviation from unit magnitude is 8.44D-15 for 2317.

Iteration 1 A^-1\*A deviation from orthogonality is 1.79D-12 for 1343 1159.

E= -1658.67695795700

DIIS: error= 3.47D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67695795700 IErMin= 1 ErrMin= 3.47D-04

ErrMax= 3.47D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.24D-05 BMatP= 6.24D-05

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.47D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 88.629 Goal= None Shift= 0.000

Gap= 88.629 Goal= None Shift= 0.000

RMSDP=1.78D-05 MaxDP=1.06D-03 OVMax= 1.59D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.78D-05 CP: 1.00D+00

E= -1658.67695407572 Delta-E= 0.000003881275 Rises=F Damp=F

DIIS: error= 3.40D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 1 EnMin= -1658.67695795700 IErMin= 2 ErrMin= 3.40D-04

ErrMax= 3.40D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.01D-04 BMatP= 6.24D-05

IDIUse=3 WtCom= 3.52D-01 WtEn= 6.48D-01

Coeff-Com: 0.570D+00 0.430D+00

Coeff-En: 0.570D+00 0.430D+00

Coeff: 0.570D+00 0.430D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.24D-05 MaxDP=8.41D-04 DE= 3.88D-06 OVMax= 1.06D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 8.16D-06 CP: 1.00D+00 4.77D-01

E= -1658.67697090652 Delta-E= -0.000016830794 Rises=F Damp=F

DIIS: error= 9.91D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67697090652 IErMin= 3 ErrMin= 9.91D-05

ErrMax= 9.91D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.31D-06 BMatP= 6.24D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.810D-01 0.216D+00 0.703D+00

Coeff: 0.810D-01 0.216D+00 0.703D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.04D-06 MaxDP=2.00D-04 DE=-1.68D-05 OVMax= 4.20D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.82D-06 CP: 1.00D+00 5.78D-01 7.22D-01

E= -1658.67697172995 Delta-E= -0.000000823428 Rises=F Damp=F

DIIS: error= 7.75D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67697172995 IErMin= 4 ErrMin= 7.75D-05

ErrMax= 7.75D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.64D-06 BMatP= 7.31D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.938D-02 0.988D-01 0.475D+00 0.436D+00

Coeff: -0.938D-02 0.988D-01 0.475D+00 0.436D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.77D-06 MaxDP=8.44D-05 DE=-8.23D-07 OVMax= 1.83D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 5.52D-07 CP: 1.00D+00 5.78D-01 8.21D-01 4.78D-01

E= -1658.67697219880 Delta-E= -0.000000468849 Rises=F Damp=F

DIIS: error= 8.36D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67697219880 IErMin= 5 ErrMin= 8.36D-06

ErrMax= 8.36D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.60D-08 BMatP= 2.64D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.899D-02 0.389D-01 0.203D+00 0.219D+00 0.548D+00

Coeff: -0.899D-02 0.389D-01 0.203D+00 0.219D+00 0.548D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.10D-07 MaxDP=1.89D-05 DE=-4.69D-07 OVMax= 2.55D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.26D-07 CP: 1.00D+00 5.80D-01 8.23D-01 4.88D-01 6.24D-01

E= -1658.67697220813 Delta-E= -0.000000009339 Rises=F Damp=F

DIIS: error= 1.30D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67697220813 IErMin= 6 ErrMin= 1.30D-06

ErrMax= 1.30D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.98D-09 BMatP= 5.60D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.261D-02 0.710D-02 0.407D-01 0.508D-01 0.233D+00 0.671D+00

Coeff: -0.261D-02 0.710D-02 0.407D-01 0.508D-01 0.233D+00 0.671D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.01D-07 MaxDP=5.47D-06 DE=-9.34D-09 OVMax= 9.51D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 7.51D-08 CP: 1.00D+00 5.81D-01 8.22D-01 4.96D-01 7.04D-01

CP: 8.17D-01

E= -1658.67697220870 Delta-E= -0.000000000563 Rises=F Damp=F

DIIS: error= 5.67D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67697220870 IErMin= 7 ErrMin= 5.67D-07

ErrMax= 5.67D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.04D-10 BMatP= 2.98D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.417D-03 0.129D-03 0.248D-02 0.518D-02 0.594D-01 0.304D+00

Coeff-Com: 0.630D+00

Coeff: -0.417D-03 0.129D-03 0.248D-02 0.518D-02 0.594D-01 0.304D+00

Coeff: 0.630D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.11D-08 MaxDP=1.91D-06 DE=-5.63D-10 OVMax= 2.91D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.79D-08 CP: 1.00D+00 5.80D-01 8.23D-01 4.97D-01 7.10D-01

CP: 8.78D-01 6.87D-01

E= -1658.67697220882 Delta-E= -0.000000000122 Rises=F Damp=F

DIIS: error= 1.66D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67697220882 IErMin= 8 ErrMin= 1.66D-07

ErrMax= 1.66D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.98D-11 BMatP= 3.04D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.125D-03-0.846D-03-0.413D-02-0.422D-02-0.275D-02 0.548D-01

Coeff-Com: 0.302D+00 0.655D+00

Coeff: 0.125D-03-0.846D-03-0.413D-02-0.422D-02-0.275D-02 0.548D-01

Coeff: 0.302D+00 0.655D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.54D-08 MaxDP=5.72D-07 DE=-1.22D-10 OVMax= 1.97D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 8.30D-09 CP: 1.00D+00 5.81D-01 8.23D-01 4.97D-01 7.15D-01

CP: 8.99D-01 8.22D-01 8.16D-01

E= -1658.67697220882 Delta-E= 0.000000000000 Rises=F Damp=F

DIIS: error= 3.12D-08 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67697220882 IErMin= 9 ErrMin= 3.12D-08

ErrMax= 3.12D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.93D-12 BMatP= 3.98D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.763D-04-0.363D-03-0.187D-02-0.205D-02-0.511D-02 0.844D-03

Coeff-Com: 0.696D-01 0.264D+00 0.675D+00

Coeff: 0.763D-04-0.363D-03-0.187D-02-0.205D-02-0.511D-02 0.844D-03

Coeff: 0.696D-01 0.264D+00 0.675D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.15D-09 MaxDP=2.99D-07 DE=-4.55D-13 OVMax= 8.89D-07

Error on total polarization charges = 0.04168

SCF Done: E(UB3LYP) = -1658.67697221 A.U. after 9 cycles

NFock= 9 Conv=0.61D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655241417528D+03 PE=-6.145877080757D+03 EE= 1.730404674312D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.64

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:43:28 2019, MaxMem= 1342177280 cpu: 224.8

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 337

Leave Link 701 at Sat Aug 17 17:43:29 2019, MaxMem= 1342177280 cpu: 10.2

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:43:29 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:43:32 2019, MaxMem= 1342177280 cpu: 36.1

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.35846727D+00-2.91171229D+00 5.95669151D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000926090 -0.000561638 0.000421050

2 6 -0.000309849 -0.000277736 0.000305817

3 8 -0.000780607 0.000625055 -0.000492242

4 8 0.000124506 -0.000076843 0.000073061

5 6 0.000111296 -0.000090848 -0.000044048

6 16 0.000087188 0.000278914 -0.000186809

7 6 -0.000104321 0.000110018 -0.000188577

8 16 0.000367535 -0.000094420 0.000060004

9 16 -0.000078295 -0.000055534 0.000248160

10 6 -0.000301424 -0.000011130 0.000005911

11 6 -0.000028795 -0.000106970 -0.000002726

12 6 -0.000076253 0.000089017 -0.000021911

13 6 0.000092494 -0.000145261 -0.000042374

14 1 0.000082038 0.000133204 -0.000057178

15 1 -0.000168939 0.000024911 -0.000098048

16 1 0.000152894 0.000021566 0.000067664

17 1 -0.000047338 0.000043754 0.000047215

18 1 -0.000042154 -0.000064501 -0.000060372

19 1 0.000130263 0.000173285 -0.000106498

20 1 -0.000106955 -0.000055189 0.000129214

21 1 -0.000036772 0.000032635 0.000083084

22 1 0.000025761 -0.000052401 -0.000096717

23 1 -0.000014328 0.000021882 -0.000039454

24 1 0.000051791 -0.000008401 0.000103262

25 1 0.000034681 0.000056838 -0.000025625

26 1 -0.000009789 -0.000036409 0.000028864

27 1 -0.000080717 0.000026203 -0.000110727

-------------------------------------------------------------------

Cartesian Forces: Max 0.000926090 RMS 0.000214300

Leave Link 716 at Sat Aug 17 17:43:32 2019, MaxMem= 1342177280 cpu: 0.3

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.001102781 RMS 0.000175155

Search for a local minimum.

Step number 30 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .17516D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 27

ITU= 0 -1 -1 0 0 -1 0 0 -1 1 -1 1 -1 1 1 -1 1 -1 1 1

ITU= -1 0 0 -1 0 0 -1 -1 0 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.84538.

Iteration 1 RMS(Cart)= 0.00593623 RMS(Int)= 0.00002228

Iteration 2 RMS(Cart)= 0.00003776 RMS(Int)= 0.00000006

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000006

ITry= 1 IFail=0 DXMaxC= 2.91D-02 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=T

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83747 -0.00004 -0.00015 0.00000 -0.00015 2.83732

R2 2.28720 0.00110 0.00049 0.00000 0.00049 2.28769

R3 2.55307 0.00010 -0.00004 0.00000 -0.00004 2.55303

R4 2.86618 0.00005 0.00036 0.00000 0.00036 2.86653

R5 3.59867 0.00011 -0.00151 0.00000 -0.00151 3.59715

R6 2.05792 0.00010 0.00003 0.00000 0.00003 2.05795

R7 1.83667 0.00017 0.00014 0.00000 0.00014 1.83682

R8 2.06115 0.00018 0.00018 0.00000 0.00018 2.06133

R9 2.06852 0.00007 0.00014 0.00000 0.00014 2.06865

R10 2.06019 0.00003 0.00005 0.00000 0.00005 2.06023

R11 3.31927 -0.00013 0.00086 0.00000 0.00086 3.32013

R12 3.38396 0.00016 0.00014 0.00000 0.00014 3.38410

R13 3.25401 0.00003 -0.00001 0.00000 -0.00001 3.25400

R14 3.47621 -0.00030 -0.00005 0.00000 -0.00005 3.47616

R15 2.88072 0.00008 0.00015 0.00000 0.00015 2.88088

R16 2.06355 0.00019 0.00009 0.00000 0.00009 2.06364

R17 2.06007 0.00004 0.00009 0.00000 0.00009 2.06016

R18 2.89416 -0.00001 0.00005 0.00000 0.00005 2.89421

R19 2.07222 0.00006 0.00005 0.00000 0.00005 2.07227

R20 2.07079 0.00010 0.00004 0.00000 0.00004 2.07083

R21 2.88569 0.00011 0.00013 0.00000 0.00013 2.88582

R22 2.07189 0.00004 0.00004 0.00000 0.00004 2.07194

R23 2.07160 0.00008 0.00005 0.00000 0.00005 2.07165

R24 2.06756 0.00006 0.00005 0.00000 0.00005 2.06760

R25 2.06906 0.00007 0.00006 0.00000 0.00006 2.06912

R26 2.06890 0.00006 0.00004 0.00000 0.00004 2.06895

A1 2.17692 0.00010 0.00036 0.00000 0.00036 2.17728

A2 1.97586 -0.00002 -0.00010 0.00000 -0.00010 1.97575

A3 2.12987 -0.00008 -0.00028 0.00000 -0.00028 2.12959

A4 2.02416 0.00001 -0.00072 0.00000 -0.00072 2.02344

A5 1.83524 0.00006 0.00216 0.00000 0.00216 1.83741

A6 1.87158 0.00008 -0.00003 0.00000 -0.00003 1.87156

A7 1.94651 -0.00003 -0.00017 0.00000 -0.00017 1.94634

A8 1.94008 -0.00002 0.00000 0.00000 0.00000 1.94008

A9 1.83346 -0.00010 -0.00123 0.00000 -0.00123 1.83223

A10 1.87304 -0.00005 0.00009 0.00000 0.00009 1.87312

A11 1.91191 0.00002 -0.00027 0.00000 -0.00027 1.91164

A12 1.92850 -0.00009 0.00014 0.00000 0.00014 1.92865

A13 1.95248 -0.00001 -0.00015 0.00000 -0.00015 1.95233

A14 1.88383 0.00001 -0.00009 0.00000 -0.00009 1.88374

A15 1.89332 0.00002 -0.00002 0.00000 -0.00002 1.89330

A16 1.89215 0.00006 0.00039 0.00000 0.00039 1.89254

A17 1.79465 -0.00081 -0.00148 0.00000 -0.00148 1.79317

A18 1.97259 -0.00027 -0.00067 0.00000 -0.00067 1.97192

A19 2.14201 0.00009 0.00000 0.00000 0.00000 2.14200

A20 2.15414 0.00008 0.00006 0.00000 0.00006 2.15420

A21 1.79316 0.00046 -0.00005 0.00000 -0.00005 1.79311

A22 1.92887 -0.00054 -0.00029 0.00000 -0.00029 1.92858

A23 1.87469 0.00027 -0.00005 0.00000 -0.00005 1.87465

A24 1.89457 0.00010 0.00045 0.00000 0.00045 1.89502

A25 1.93897 0.00008 -0.00026 0.00000 -0.00026 1.93871

A26 1.93826 0.00014 0.00012 0.00000 0.00012 1.93838

A27 1.88647 -0.00004 0.00004 0.00000 0.00004 1.88652

A28 1.95228 0.00023 0.00010 0.00000 0.00010 1.95239

A29 1.91780 -0.00013 0.00013 0.00000 0.00013 1.91793

A30 1.91570 -0.00003 -0.00031 0.00000 -0.00031 1.91539

A31 1.90609 -0.00002 -0.00006 0.00000 -0.00006 1.90603

A32 1.91025 -0.00013 -0.00004 0.00000 -0.00004 1.91022

A33 1.85935 0.00006 0.00018 0.00000 0.00018 1.85953

A34 1.96734 -0.00016 -0.00005 0.00000 -0.00005 1.96729

A35 1.90669 0.00002 -0.00019 0.00000 -0.00019 1.90651

A36 1.90667 0.00009 0.00012 0.00000 0.00012 1.90680

A37 1.91300 0.00004 -0.00012 0.00000 -0.00012 1.91288

A38 1.91264 0.00003 0.00004 0.00000 0.00004 1.91268

A39 1.85404 0.00000 0.00021 0.00000 0.00021 1.85424

A40 1.94543 -0.00002 -0.00014 0.00000 -0.00014 1.94529

A41 1.94242 -0.00001 -0.00007 0.00000 -0.00007 1.94236

A42 1.94381 -0.00011 -0.00010 0.00000 -0.00010 1.94372

A43 1.87639 0.00002 0.00004 0.00000 0.00004 1.87643

A44 1.87676 0.00006 0.00018 0.00000 0.00018 1.87694

A45 1.87557 0.00006 0.00010 0.00000 0.00010 1.87566

D1 2.68311 -0.00002 -0.01400 0.00000 -0.01400 2.66911

D2 -1.44115 -0.00001 -0.01302 0.00000 -0.01302 -1.45417

D3 0.50397 -0.00007 -0.01346 0.00000 -0.01346 0.49051

D4 -0.49337 0.00004 -0.01483 0.00000 -0.01483 -0.50819

D5 1.66555 0.00006 -0.01385 0.00000 -0.01385 1.65170

D6 -2.67251 0.00000 -0.01429 0.00000 -0.01429 -2.68680

D7 -3.10269 -0.00006 -0.00040 0.00000 -0.00040 -3.10310

D8 0.00508 0.00000 -0.00119 0.00000 -0.00119 0.00389

D9 -3.12179 -0.00002 0.00222 0.00000 0.00222 -3.11957

D10 -1.04857 -0.00005 0.00202 0.00000 0.00202 -1.04655

D11 1.06133 -0.00005 0.00252 0.00000 0.00252 1.06385

D12 1.06153 -0.00008 -0.00001 0.00000 -0.00001 1.06152

D13 3.13475 -0.00012 -0.00020 0.00000 -0.00020 3.13455

D14 -1.03853 -0.00011 0.00029 0.00000 0.00029 -1.03824

D15 -0.97823 0.00008 0.00162 0.00000 0.00162 -0.97661

D16 1.09499 0.00004 0.00143 0.00000 0.00143 1.09642

D17 -3.07830 0.00005 0.00193 0.00000 0.00193 -3.07637

D18 -3.13646 0.00026 -0.00882 0.00000 -0.00882 3.13791

D19 -0.92889 0.00029 -0.00833 0.00000 -0.00833 -0.93721

D20 1.17459 0.00019 -0.00917 0.00000 -0.00917 1.16542

D21 1.84660 -0.00036 -0.00011 0.00000 -0.00011 1.84649

D22 -1.11865 0.00026 0.00352 0.00000 0.00352 -1.11513

D23 2.54938 0.00033 0.00083 0.00000 0.00083 2.55021

D24 -0.76996 -0.00029 -0.00284 0.00000 -0.00284 -0.77280

D25 -2.99818 -0.00009 0.00391 0.00000 0.00391 -2.99427

D26 -0.88042 -0.00015 0.00339 0.00000 0.00339 -0.87703

D27 1.15540 0.00001 0.00365 0.00000 0.00365 1.15905

D28 -3.10293 0.00000 -0.00027 0.00000 -0.00027 -3.10320

D29 -0.98284 0.00004 -0.00019 0.00000 -0.00019 -0.98304

D30 1.05636 0.00003 -0.00008 0.00000 -0.00008 1.05628

D31 1.10103 -0.00004 0.00014 0.00000 0.00014 1.10117

D32 -3.06208 0.00000 0.00022 0.00000 0.00022 -3.06185

D33 -1.02288 -0.00001 0.00034 0.00000 0.00034 -1.02254

D34 -0.99922 -0.00014 0.00018 0.00000 0.00018 -0.99904

D35 1.12086 -0.00010 0.00026 0.00000 0.00026 1.12112

D36 -3.12313 -0.00012 0.00037 0.00000 0.00037 -3.12275

D37 -3.13054 0.00001 0.00224 0.00000 0.00224 -3.12830

D38 -0.99936 -0.00004 0.00191 0.00000 0.00191 -0.99744

D39 1.02194 0.00002 0.00213 0.00000 0.00213 1.02406

D40 1.02582 0.00003 0.00205 0.00000 0.00205 1.02787

D41 -3.12618 -0.00002 0.00173 0.00000 0.00173 -3.12445

D42 -1.10489 0.00004 0.00194 0.00000 0.00194 -1.10295

D43 -1.00351 0.00004 0.00188 0.00000 0.00188 -1.00162

D44 1.12768 0.00000 0.00156 0.00000 0.00156 1.12924

D45 -3.13422 0.00005 0.00177 0.00000 0.00177 -3.13244

D46 -3.13840 -0.00004 -0.00056 0.00000 -0.00056 -3.13897

D47 -1.04377 -0.00003 -0.00065 0.00000 -0.00065 -1.04442

D48 1.04873 -0.00003 -0.00063 0.00000 -0.00063 1.04810

D49 1.01716 0.00002 -0.00020 0.00000 -0.00020 1.01696

D50 3.11180 0.00003 -0.00029 0.00000 -0.00029 3.11151

D51 -1.07889 0.00002 -0.00028 0.00000 -0.00028 -1.07916

D52 -1.01106 -0.00002 -0.00041 0.00000 -0.00041 -1.01147

D53 1.08358 -0.00001 -0.00049 0.00000 -0.00049 1.08308

D54 -3.10711 -0.00001 -0.00048 0.00000 -0.00048 -3.10759

Item Value Threshold Converged?

Maximum Force 0.001103 0.000450 NO

RMS Force 0.000175 0.000300 YES

Maximum Displacement 0.029055 0.001800 NO

RMS Displacement 0.005943 0.001200 NO

Predicted change in Energy=-8.056239D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:43:32 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.106011 -0.411795 -0.202789

2 6 0 -2.839946 0.059692 0.452284

3 8 0 -4.887865 0.303524 -0.788072

4 8 0 -4.283197 -1.748459 -0.118247

5 6 0 -2.345781 -0.774992 1.618517

6 16 0 -1.550804 0.137931 -0.946081

7 6 0 -0.109041 0.698445 -0.113035

8 16 0 1.105954 -0.594677 0.128916

9 16 0 -0.007955 2.246758 0.633681

10 6 0 2.699082 0.313858 -0.013518

11 6 0 3.869759 -0.662281 -0.040886

12 6 0 5.216619 0.064045 -0.104610

13 6 0 6.402956 -0.896405 -0.151579

14 1 0 -2.996664 1.095745 0.748931

15 1 0 -5.102162 -1.962626 -0.595968

16 1 0 -1.438215 -0.328960 2.027465

17 1 0 -3.096065 -0.802936 2.415152

18 1 0 -2.122718 -1.799241 1.318932

19 1 0 2.657912 0.903639 -0.931665

20 1 0 2.782655 1.002355 0.827611

21 1 0 3.845266 -1.299317 0.851366

22 1 0 3.774420 -1.330561 -0.904121

23 1 0 5.234834 0.714489 -0.987066

24 1 0 5.312627 0.724491 0.765106

25 1 0 7.353618 -0.356444 -0.194036

26 1 0 6.428798 -1.539870 0.733948

27 1 0 6.354085 -1.548046 -1.030015

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.501447 0.000000

3 O 1.210592 2.406639 0.000000

4 O 1.351004 2.382832 2.241634 0.000000

5 C 2.558804 1.516903 3.662930 2.778051 0.000000

6 S 2.717308 1.903531 3.344901 3.421951 2.835944

7 C 4.149271 2.861019 4.842395 4.838486 3.189403

8 S 5.225710 4.012841 6.129722 5.516815 3.763761

9 S 4.955971 3.582783 5.441605 5.899564 3.945416

10 C 6.846290 5.564387 7.626389 7.281232 5.412926

11 C 7.981344 6.766432 8.842344 8.225355 6.434226

12 C 9.335282 8.075791 10.130404 9.671188 7.801477

13 C 10.520259 9.311821 11.372229 10.720121 8.926835

14 H 2.099785 1.089020 2.562544 3.239855 2.163211

15 H 1.884671 3.210331 2.284351 0.972002 3.729887

16 H 3.478222 2.144083 4.497485 3.835750 1.090807

17 H 2.833125 2.159299 3.833463 2.953202 1.094685

18 H 2.859037 2.172815 4.062896 2.595329 1.090227

19 H 6.929089 5.731841 7.570965 7.474909 5.861584

20 H 7.107409 5.713416 7.869922 7.641197 5.485012

21 H 8.069804 6.833610 9.029088 8.198401 6.260391

22 H 7.964747 6.893655 8.815832 8.106629 6.642983

23 H 9.441133 8.228156 10.132992 9.869847 8.153119

24 H 9.536179 8.185613 10.326646 9.948650 7.850349

25 H 11.459766 10.222507 12.273645 11.720023 9.876177

26 H 10.636363 9.409970 11.566395 10.747864 8.852160

27 H 10.554097 9.450515 11.395977 10.678167 9.126883

6 7 8 9 10

6 S 0.000000

7 C 1.756935 0.000000

8 S 2.958158 1.790787 0.000000

9 S 3.053389 1.721940 3.093435 0.000000

10 C 4.354556 2.836083 1.839506 3.388660 0.000000

11 C 5.553577 4.205667 2.769841 4.894305 1.524494

12 C 6.819938 5.363320 4.169655 5.710122 2.531541

13 C 8.059987 6.704562 5.312998 7.183028 3.899036

14 H 2.425075 3.039605 4.480337 3.204762 5.799500

15 H 4.140901 5.678536 6.398238 6.721748 8.147456

16 H 3.012082 2.721029 3.185575 3.259233 4.657901

17 H 3.817191 4.191442 4.788237 4.691556 6.381959

18 H 3.034799 3.513382 3.645742 4.616482 5.430503

19 H 4.277827 2.892800 2.403821 3.370627 1.092030

20 H 4.761521 3.055992 2.418680 3.061642 1.090188

21 H 5.866350 4.534056 2.919295 5.241121 2.159652

22 H 5.524151 4.452410 2.954556 5.428481 2.157230

23 H 6.810212 5.414905 4.472917 5.697500 2.745604

24 H 7.097810 5.492386 4.454329 5.535627 2.757806

25 H 8.949789 7.537284 6.260540 7.852041 4.706018

26 H 8.325356 6.962096 5.439864 7.468627 4.231524

27 H 8.083120 6.903591 5.458471 7.592363 4.225991

11 12 13 14 15

11 C 0.000000

12 C 1.531550 0.000000

13 C 2.546401 1.527110 0.000000

14 H 7.131777 8.321717 9.650516 0.000000

15 H 9.082642 10.527397 11.562961 3.949115 0.000000

16 H 5.706467 6.999072 8.158075 2.468440 4.793305

17 H 7.387463 8.729352 9.840135 2.528074 3.799493

18 H 6.249125 7.704815 8.698542 3.077276 3.545507

19 H 2.171213 2.817077 4.227771 5.902164 8.279306

20 H 2.169585 2.770134 4.203651 5.780609 8.543303

21 H 1.096599 2.157141 2.776692 7.249746 9.087971

22 H 1.095838 2.159649 2.768395 7.380185 8.904391

23 H 2.157356 1.096421 2.158131 8.421200 10.685195

24 H 2.157459 1.096272 2.157877 8.317597 10.841631

25 H 3.500610 2.179810 1.094129 10.494112 12.565343

26 H 2.814109 2.178325 1.094931 9.787034 11.615095

27 H 2.816883 2.179229 1.094839 9.878805 11.471960

16 17 18 19 20

16 H 0.000000

17 H 1.767321 0.000000

18 H 1.769828 1.772492 0.000000

19 H 5.201346 6.871814 5.935079 0.000000

20 H 4.585607 6.351277 5.670363 1.766453 0.000000

21 H 5.499088 7.132594 6.007110 3.072787 2.535232

22 H 6.063742 7.648499 6.319641 2.497798 3.070015

23 H 7.396334 9.125873 8.109873 2.584449 3.064164

24 H 6.948178 8.704125 7.871487 3.155731 2.545953

25 H 9.068194 10.779755 9.704210 4.917476 4.876864

26 H 8.064079 9.700131 8.575424 4.792137 4.445902

27 H 8.458976 10.086114 8.799820 4.436454 4.765546

21 22 23 24 25

21 H 0.000000

22 H 1.757194 0.000000

23 H 3.060416 2.514343 0.000000

24 H 2.501278 3.061967 1.753927 0.000000

25 H 3.780266 3.776743 2.503007 2.500804 0.000000

26 H 2.597362 3.126148 3.077267 2.524706 1.765487

27 H 3.145733 2.591875 2.524605 3.077583 1.765741

26 27

26 H 0.000000

27 H 1.765563 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 4.10D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.117527 -0.425223 -0.158256

2 6 0 -2.845962 0.114153 0.430417

3 8 0 -4.900130 0.220119 -0.819012

4 8 0 -4.299128 -1.742051 0.082991

5 6 0 -2.348111 -0.580553 1.683623

6 16 0 -1.564672 0.022752 -0.974351

7 6 0 -0.116054 0.670596 -0.220279

8 16 0 1.095567 -0.590603 0.164780

9 16 0 -0.004954 2.295157 0.339667

10 6 0 2.691168 0.288143 -0.091429

11 6 0 3.858074 -0.689554 -0.010676

12 6 0 5.207200 0.018505 -0.166093

13 6 0 6.389710 -0.945971 -0.106725

14 1 0 -2.997152 1.178456 0.604679

15 1 0 -5.121630 -2.007069 -0.362030

16 1 0 -1.436557 -0.093688 2.032751

17 1 0 -3.093861 -0.511900 2.482046

18 1 0 -2.130552 -1.633764 1.504709

19 1 0 2.646840 0.766681 -1.072025

20 1 0 2.782145 1.069911 0.662939

21 1 0 3.836415 -1.217765 0.950079

22 1 0 3.755277 -1.453777 -0.789301

23 1 0 5.222686 0.561206 -1.118656

24 1 0 5.310675 0.775704 0.619880

25 1 0 7.342086 -0.418796 -0.217112

26 1 0 6.418322 -1.481572 0.847835

27 1 0 6.333352 -1.695648 -0.902640

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3276612 0.1920518 0.1800601

Leave Link 202 at Sat Aug 17 17:43:32 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1101.6017521090 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0549318167 Hartrees.

Nuclear repulsion after empirical dispersion term = 1101.5468202923 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2318

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.56D-07

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 102

GePol: Fraction of low-weight points (<1% of avg) = 4.40%

GePol: Cavity surface area = 309.419 Ang\*\*2

GePol: Cavity volume = 320.168 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057975813 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1101.5410227110 Hartrees.

Leave Link 301 at Sat Aug 17 17:43:32 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:43:32 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:43:32 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Lowest energy guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000116 0.000002 0.000022 Ang= 0.01 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000655 -0.000014 -0.000119 Ang= -0.08 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 1.55D-01

Max alpha theta= 0.574 degrees.

Max beta theta= 0.582 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 17:43:33 2019, MaxMem= 1342177280 cpu: 4.3

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16119372.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.11D-15 for 2318.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.68D-15 for 678 467.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.11D-15 for 2318.

Iteration 1 A^-1\*A deviation from orthogonality is 9.10D-13 for 917 910.

E= -1658.67697559226

DIIS: error= 2.12D-06 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67697559226 IErMin= 1 ErrMin= 2.12D-06

ErrMax= 2.12D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.32D-09 BMatP= 2.32D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 88.617 Goal= None Shift= 0.000

Gap= 88.622 Goal= None Shift= 0.000

RMSDP=1.07D-07 MaxDP=6.35D-06 OVMax= 9.75D-06

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.07D-07 CP: 1.00D+00

E= -1658.67697559214 Delta-E= 0.000000000122 Rises=F Damp=F

DIIS: error= 2.12D-06 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 1 EnMin= -1658.67697559226 IErMin= 2 ErrMin= 2.12D-06

ErrMax= 2.12D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.53D-09 BMatP= 2.32D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.560D+00 0.440D+00

Coeff: 0.560D+00 0.440D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=7.32D-08 MaxDP=5.08D-06 DE= 1.22D-10 OVMax= 6.52D-06

Cycle 3 Pass 1 IDiag 1:

RMSU= 4.94D-08 CP: 1.00D+00 4.97D-01

E= -1658.67697559272 Delta-E= -0.000000000583 Rises=F Damp=F

DIIS: error= 5.21D-07 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67697559272 IErMin= 3 ErrMin= 5.21D-07

ErrMax= 5.21D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.57D-10 BMatP= 2.32D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.685D-01 0.216D+00 0.716D+00

Coeff: 0.685D-01 0.216D+00 0.716D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.41D-08 MaxDP=1.20D-06 DE=-5.83D-10 OVMax= 2.47D-06

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.70D-08 CP: 1.00D+00 5.97D-01 7.32D-01

E= -1658.67697559279 Delta-E= -0.000000000067 Rises=F Damp=F

DIIS: error= 4.75D-07 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67697559279 IErMin= 4 ErrMin= 4.75D-07

ErrMax= 4.75D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.60D-11 BMatP= 2.57D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.903D-02 0.104D+00 0.485D+00 0.420D+00

Coeff: -0.903D-02 0.104D+00 0.485D+00 0.420D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.08D-08 MaxDP=4.78D-07 DE=-6.73D-11 OVMax= 1.16D-06

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.45D-09 CP: 1.00D+00 5.97D-01 8.26D-01 4.64D-01

E= -1658.67697559275 Delta-E= 0.000000000037 Rises=F Damp=F

DIIS: error= 5.21D-08 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 4 EnMin= -1658.67697559279 IErMin= 5 ErrMin= 5.21D-08

ErrMax= 5.21D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.12D-12 BMatP= 9.60D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.876D-02 0.403D-01 0.205D+00 0.212D+00 0.552D+00

Coeff: -0.876D-02 0.403D-01 0.205D+00 0.212D+00 0.552D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.90D-09 MaxDP=1.15D-07 DE= 3.68D-11 OVMax= 1.51D-07

Error on total polarization charges = 0.04168

SCF Done: E(UB3LYP) = -1658.67697559 A.U. after 5 cycles

NFock= 5 Conv=0.19D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655239726306D+03 PE=-6.145848817696D+03 EE= 1.730391093086D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.64

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:43:45 2019, MaxMem= 1342177280 cpu: 137.1

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 338

Leave Link 701 at Sat Aug 17 17:43:46 2019, MaxMem= 1342177280 cpu: 10.3

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:43:46 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:43:49 2019, MaxMem= 1342177280 cpu: 38.4

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.36280912D+00-2.91260014D+00 5.91154554D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000661323 -0.000354768 -0.000001129

2 6 -0.000310305 -0.000201025 0.000409554

3 8 -0.000516114 0.000424242 -0.000239535

4 8 0.000062029 -0.000100567 0.000116259

5 6 0.000142831 -0.000037446 -0.000037255

6 16 0.000131902 0.000286140 -0.000188265

7 6 -0.000120135 0.000052916 -0.000181060

8 16 0.000361592 -0.000049750 0.000034973

9 16 -0.000052437 -0.000056310 0.000222709

10 6 -0.000254387 -0.000015489 -0.000020538

11 6 -0.000025464 -0.000075938 0.000013033

12 6 -0.000071799 0.000061842 -0.000052261

13 6 0.000056281 -0.000111024 -0.000011742

14 1 0.000029400 0.000073801 -0.000017827

15 1 -0.000100356 0.000033523 -0.000048969

16 1 0.000103090 -0.000018248 0.000059556

17 1 -0.000029403 0.000025349 0.000017695

18 1 -0.000058689 -0.000055950 -0.000041369

19 1 0.000119183 0.000159790 -0.000075364

20 1 -0.000115326 -0.000070813 0.000112072

21 1 -0.000046255 0.000030087 0.000059502

22 1 0.000033942 -0.000051428 -0.000072323

23 1 -0.000005164 0.000025834 -0.000020881

24 1 0.000041980 -0.000010276 0.000074169

25 1 0.000026995 0.000034407 -0.000027655

26 1 -0.000002818 -0.000031282 0.000008129

27 1 -0.000061898 0.000032384 -0.000091481

-------------------------------------------------------------------

Cartesian Forces: Max 0.000661323 RMS 0.000159407

Leave Link 716 at Sat Aug 17 17:43:49 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000692400 RMS 0.000140022

Search for a local minimum.

Step number 31 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .14002D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 27 30

31

ITU= 0 0 -1 -1 0 0 -1 0 0 -1 1 -1 1 -1 1 1 -1 1 -1 1

ITU= 1 -1 0 0 -1 0 0 -1 -1 0 0

Eigenvalues --- 0.00000 0.00101 0.00175 0.00266 0.00387

Eigenvalues --- 0.00419 0.00551 0.00880 0.01076 0.01954

Eigenvalues --- 0.02348 0.03535 0.03673 0.04054 0.04460

Eigenvalues --- 0.04777 0.04856 0.05155 0.05385 0.05465

Eigenvalues --- 0.05497 0.05593 0.05826 0.05901 0.08010

Eigenvalues --- 0.08241 0.08385 0.11034 0.11751 0.12231

Eigenvalues --- 0.13337 0.14521 0.15396 0.15971 0.16003

Eigenvalues --- 0.16057 0.16168 0.16263 0.16373 0.17451

Eigenvalues --- 0.18950 0.19854 0.21900 0.22088 0.22385

Eigenvalues --- 0.24263 0.24423 0.25364 0.26115 0.26841

Eigenvalues --- 0.27045 0.28253 0.29044 0.29183 0.29544

Eigenvalues --- 0.29938 0.30243 0.32032 0.33714 0.33861

Eigenvalues --- 0.33876 0.33906 0.33948 0.34023 0.34037

Eigenvalues --- 0.34114 0.34137 0.34297 0.34444 0.34557

Eigenvalues --- 0.34709 0.37449 0.52680 0.54849 0.95903

Eigenvalue 1 is 2.27D-06 Eigenvector:

D26 D25 D27 D1 D2

1 0.38912 0.38669 0.37046 0.27173 0.26532

D3 D4 D5 D6 D34

1 0.24739 0.18113 0.17473 0.15680 0.13106

En-DIIS/RFO-DIIS IScMMF= 0 using points: 31 30

RFO step: Lambda=-1.19448646D-05.

NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=F DC= 3.38D-06 SmlDif= 1.00D-05

RMS Error= 0.2005737786D-02 NUsed= 2 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: -1.95611 2.95611

Iteration 1 RMS(Cart)= 0.29254828 RMS(Int)= 0.11729931

Iteration 2 RMS(Cart)= 0.18873778 RMS(Int)= 0.07041231

Iteration 3 RMS(Cart)= 0.14354122 RMS(Int)= 0.03729670

Iteration 4 RMS(Cart)= 0.13734353 RMS(Int)= 0.00762219

Iteration 5 RMS(Cart)= 0.02822256 RMS(Int)= 0.00170130

Iteration 6 RMS(Cart)= 0.00028853 RMS(Int)= 0.00169216

Iteration 7 RMS(Cart)= 0.00000010 RMS(Int)= 0.00169216

ITry= 1 IFail=0 DXMaxC= 2.71D+00 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83732 -0.00001 0.00043 0.01506 0.01549 2.85281

R2 2.28769 0.00069 -0.00144 0.00829 0.00685 2.29454

R3 2.55303 0.00012 0.00011 0.01286 0.01297 2.56600

R4 2.86653 0.00004 -0.00105 0.00850 0.00745 2.87398

R5 3.59715 0.00019 0.00448 0.01538 0.01986 3.61701

R6 2.05795 0.00006 -0.00010 -0.00310 -0.00320 2.05475

R7 1.83682 0.00009 -0.00043 0.00259 0.00217 1.83898

R8 2.06133 0.00012 -0.00053 -0.00311 -0.00364 2.05769

R9 2.06865 0.00004 -0.00040 0.00458 0.00418 2.07283

R10 2.06023 0.00002 -0.00014 0.00170 0.00156 2.06180

R11 3.32013 -0.00015 -0.00254 0.03373 0.03120 3.35132

R12 3.38410 0.00014 -0.00042 0.00596 0.00554 3.38964

R13 3.25400 0.00002 0.00004 0.00498 0.00501 3.25901

R14 3.47616 -0.00029 0.00014 -0.02497 -0.02484 3.45132

R15 2.88088 0.00005 -0.00046 0.00889 0.00844 2.88931

R16 2.06364 0.00015 -0.00026 0.01123 0.01097 2.07461

R17 2.06016 0.00002 -0.00026 0.00253 0.00226 2.06242

R18 2.89421 -0.00002 -0.00016 -0.00092 -0.00108 2.89313

R19 2.07227 0.00005 -0.00015 0.00426 0.00410 2.07637

R20 2.07083 0.00008 -0.00012 0.00583 0.00571 2.07654

R21 2.88582 0.00008 -0.00038 0.00974 0.00936 2.89518

R22 2.07194 0.00003 -0.00013 0.00157 0.00144 2.07337

R23 2.07165 0.00005 -0.00016 0.00427 0.00412 2.07577

R24 2.06760 0.00004 -0.00014 0.00314 0.00300 2.07060

R25 2.06912 0.00005 -0.00017 0.00386 0.00369 2.07281

R26 2.06895 0.00004 -0.00013 0.00285 0.00272 2.07166

A1 2.17728 0.00009 -0.00106 0.00922 0.00290 2.18017

A2 1.97575 -0.00009 0.00031 -0.01132 -0.01627 1.95948

A3 2.12959 0.00000 0.00083 0.00801 0.00353 2.13312

A4 2.02344 0.00001 0.00213 -0.05965 -0.05790 1.96554

A5 1.83741 -0.00001 -0.00640 0.03299 0.02696 1.86437

A6 1.87156 0.00007 0.00008 -0.00002 -0.00106 1.87050

A7 1.94634 0.00002 0.00049 0.02059 0.02145 1.96780

A8 1.94008 -0.00003 0.00000 -0.00378 -0.00475 1.93532

A9 1.83223 -0.00007 0.00363 0.01803 0.02147 1.85370

A10 1.87312 -0.00004 -0.00026 0.04325 0.04299 1.91611

A11 1.91164 0.00005 0.00081 0.00799 0.00869 1.92033

A12 1.92865 -0.00009 -0.00042 -0.02482 -0.02527 1.90338

A13 1.95233 0.00000 0.00045 0.00681 0.00713 1.95946

A14 1.88374 0.00000 0.00026 -0.00324 -0.00299 1.88075

A15 1.89330 0.00001 0.00005 0.01586 0.01570 1.90900

A16 1.89254 0.00004 -0.00116 -0.00232 -0.00353 1.88901

A17 1.79317 -0.00056 0.00438 0.02873 0.03311 1.82628

A18 1.97192 -0.00022 0.00198 -0.02875 -0.03563 1.93629

A19 2.14200 0.00009 0.00001 0.00764 -0.00185 2.14016

A20 2.15420 0.00004 -0.00018 -0.02122 -0.03028 2.12392

A21 1.79311 0.00044 0.00014 0.04945 0.04958 1.84270

A22 1.92858 -0.00050 0.00085 -0.07822 -0.07765 1.85094

A23 1.87465 0.00025 0.00014 0.03705 0.03738 1.91203

A24 1.89502 0.00008 -0.00132 0.00163 -0.00057 1.89444

A25 1.93871 0.00010 0.00078 0.01571 0.01676 1.95547

A26 1.93838 0.00012 -0.00036 0.01015 0.00889 1.94727

A27 1.88652 -0.00004 -0.00013 0.01622 0.01564 1.90216

A28 1.95239 0.00022 -0.00030 0.04908 0.04874 2.00112

A29 1.91793 -0.00014 -0.00038 -0.02080 -0.02181 1.89612

A30 1.91539 0.00000 0.00092 -0.01151 -0.01038 1.90501

A31 1.90603 -0.00001 0.00018 0.00976 0.00995 1.91599

A32 1.91022 -0.00013 0.00010 -0.02672 -0.02644 1.88378

A33 1.85953 0.00005 -0.00054 -0.00240 -0.00312 1.85641

A34 1.96729 -0.00015 0.00015 -0.02757 -0.02765 1.93964

A35 1.90651 0.00003 0.00055 -0.00813 -0.00817 1.89833

A36 1.90680 0.00008 -0.00037 0.02951 0.02927 1.93606

A37 1.91288 0.00004 0.00036 -0.01145 -0.01157 1.90131

A38 1.91268 0.00002 -0.00013 0.01024 0.01037 1.92306

A39 1.85424 -0.00001 -0.00061 0.00969 0.00913 1.86337

A40 1.94529 0.00000 0.00042 0.00887 0.00929 1.95458

A41 1.94236 0.00000 0.00020 0.00037 0.00053 1.94288

A42 1.94372 -0.00009 0.00028 -0.01826 -0.01797 1.92574

A43 1.87643 0.00001 -0.00012 0.00077 0.00062 1.87706

A44 1.87694 0.00004 -0.00054 0.00312 0.00262 1.87956

A45 1.87566 0.00005 -0.00029 0.00572 0.00540 1.88106

D1 2.66911 -0.00005 0.04138 -0.54579 -0.50393 2.16518

D2 -1.45417 -0.00002 0.03849 -0.53289 -0.49437 -1.94855

D3 0.49051 -0.00007 0.03979 -0.49806 -0.45822 0.03228

D4 -0.50819 0.00008 0.04383 -0.35993 -0.31599 -0.82418

D5 1.65170 0.00010 0.04094 -0.34703 -0.30643 1.34528

D6 -2.68680 0.00006 0.04224 -0.31220 -0.27028 -2.95708

D7 -3.10310 -0.00010 0.00119 -0.14751 -0.14614 3.03395

D8 0.00389 0.00003 0.00352 0.03264 0.03598 0.03987

D9 -3.11957 -0.00003 -0.00655 -0.06178 -0.06856 3.09506

D10 -1.04655 -0.00005 -0.00598 -0.07594 -0.08222 -1.12876

D11 1.06385 -0.00007 -0.00745 -0.09145 -0.09922 0.96463

D12 1.06152 -0.00004 0.00004 -0.07796 -0.07779 0.98373

D13 3.13455 -0.00007 0.00060 -0.09213 -0.09145 3.04309

D14 -1.03824 -0.00008 -0.00086 -0.10764 -0.10845 -1.14670

D15 -0.97661 0.00005 -0.00480 -0.11107 -0.11563 -1.09224

D16 1.09642 0.00003 -0.00423 -0.12524 -0.12929 0.96713

D17 -3.07637 0.00001 -0.00569 -0.14075 -0.14629 3.06053

D18 3.13791 0.00025 0.02608 -0.18136 -0.15528 2.98263

D19 -0.93721 0.00027 0.02461 -0.21986 -0.19527 -1.13248

D20 1.16542 0.00020 0.02711 -0.20215 -0.17503 0.99039

D21 1.84649 -0.00031 0.00033 -0.17412 -0.17308 1.67342

D22 -1.11513 0.00022 -0.01042 0.07877 0.06764 -1.04749

D23 2.55021 0.00029 -0.00245 0.11599 0.11057 2.66078

D24 -0.77280 -0.00024 0.00840 -0.13553 -0.12416 -0.89696

D25 -2.99427 -0.00013 -0.01156 -0.81819 -0.82904 2.45988

D26 -0.87703 -0.00015 -0.01002 -0.82221 -0.83268 -1.70971

D27 1.15905 -0.00002 -0.01079 -0.78253 -0.79358 0.36547

D28 -3.10320 0.00001 0.00080 -0.24030 -0.23957 2.94042

D29 -0.98304 0.00006 0.00056 -0.20944 -0.20925 -1.19228

D30 1.05628 0.00003 0.00023 -0.23128 -0.23119 0.82509

D31 1.10117 -0.00004 -0.00042 -0.24591 -0.24610 0.85507

D32 -3.06185 0.00000 -0.00066 -0.21504 -0.21578 3.00555

D33 -1.02254 -0.00002 -0.00099 -0.23689 -0.23772 -1.26026

D34 -0.99904 -0.00014 -0.00054 -0.28379 -0.28411 -1.28315

D35 1.12112 -0.00010 -0.00077 -0.25292 -0.25379 0.86733

D36 -3.12275 -0.00012 -0.00111 -0.27477 -0.27572 2.88471

D37 -3.12830 -0.00001 -0.00661 0.17508 0.16863 -2.95968

D38 -0.99744 -0.00005 -0.00565 0.13607 0.13078 -0.86667

D39 1.02406 0.00000 -0.00628 0.15957 0.15364 1.17770

D40 1.02787 0.00002 -0.00606 0.16226 0.15586 1.18373

D41 -3.12445 -0.00001 -0.00510 0.12325 0.11800 -3.00645

D42 -1.10295 0.00003 -0.00573 0.14675 0.14087 -0.96208

D43 -1.00162 0.00004 -0.00557 0.17466 0.16888 -0.83274

D44 1.12924 0.00000 -0.00462 0.13565 0.13103 1.26027

D45 -3.13244 0.00005 -0.00525 0.15914 0.15389 -2.97855

D46 -3.13897 -0.00003 0.00167 -0.11989 -0.11812 3.02610

D47 -1.04442 -0.00002 0.00192 -0.11265 -0.11061 -1.15503

D48 1.04810 -0.00002 0.00188 -0.11746 -0.11545 0.93265

D49 1.01696 0.00001 0.00060 -0.08255 -0.08210 0.93486

D50 3.11151 0.00002 0.00086 -0.07532 -0.07459 3.03692

D51 -1.07916 0.00002 0.00081 -0.08013 -0.07942 -1.15859

D52 -1.01147 -0.00002 0.00121 -0.09355 -0.09235 -1.10381

D53 1.08308 0.00000 0.00146 -0.08631 -0.08484 0.99825

D54 -3.10759 -0.00001 0.00142 -0.09112 -0.08967 3.08593

Item Value Threshold Converged?

Maximum Force 0.000692 0.000450 NO

RMS Force 0.000140 0.000300 YES

Maximum Displacement 2.713048 0.001800 NO

RMS Displacement 0.693618 0.001200 NO

Predicted change in Energy=-4.474313D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:43:49 2019, MaxMem= 1342177280 cpu: 0.6

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.072225 -0.271163 0.233061

2 6 0 -2.633365 -0.076409 0.646314

3 8 0 -5.008727 0.381095 0.647611

4 8 0 -4.244673 -1.387731 -0.520158

5 6 0 -2.005573 -1.347801 1.196230

6 16 0 -1.705496 0.605789 -0.882480

7 6 0 -0.106469 1.064978 -0.268183

8 16 0 1.085974 -0.246998 -0.540626

9 16 0 0.109597 2.242221 0.973442

10 6 0 2.707548 0.583204 -0.670469

11 6 0 3.704215 -0.319769 0.056860

12 6 0 5.174839 0.043959 -0.164193

13 6 0 6.101690 -1.048134 0.379410

14 1 0 -2.617476 0.716756 1.389895

15 1 0 -5.193137 -1.531451 -0.683797

16 1 0 -0.958021 -1.172737 1.436346

17 1 0 -2.519087 -1.628473 2.123972

18 1 0 -2.082270 -2.182397 0.497683

19 1 0 2.968394 0.716449 -1.728510

20 1 0 2.634465 1.563628 -0.196600

21 1 0 3.474420 -0.302689 1.131195

22 1 0 3.558834 -1.357380 -0.274379

23 1 0 5.352234 0.158081 -1.240908

24 1 0 5.414205 1.010075 0.300478

25 1 0 7.150906 -0.859193 0.126344

26 1 0 6.033094 -1.122121 1.471644

27 1 0 5.828267 -2.023425 -0.039956

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.509644 0.000000

3 O 1.214219 2.419020 0.000000

4 O 1.357867 2.382547 2.253045 0.000000

5 C 2.521487 1.520845 3.508419 2.821551 0.000000

6 S 2.759507 1.914039 3.647328 3.248509 2.868378

7 C 4.214704 2.919636 5.033737 4.817053 3.401853

8 S 5.215956 3.907866 6.241138 5.451375 3.712964

9 S 4.934866 3.606509 5.455933 5.862343 4.172750

10 C 6.892868 5.540249 7.830651 7.227762 5.424652

11 C 7.778588 6.369585 8.761026 8.041039 5.912419

12 C 9.260956 7.851080 10.221434 9.534340 7.439493

13 C 10.204589 8.792990 11.205177 10.390946 8.153815

14 H 2.104885 1.087326 2.526210 3.274895 2.162019

15 H 1.919739 3.230909 2.337624 0.973149 3.705239

16 H 3.458178 2.152408 4.409616 3.830954 1.088883

17 H 2.798227 2.146027 3.523678 3.166548 1.096895

18 H 2.771780 2.181967 3.893343 2.518626 1.091055

19 H 7.375192 6.135807 8.330240 7.610258 6.128261

20 H 6.966401 5.581242 7.780068 7.492512 5.652109

21 H 7.599966 6.131178 8.524388 7.967978 5.579140

22 H 7.724664 6.389984 8.790647 7.807435 5.755467

23 H 9.548679 8.208922 10.534029 9.747289 7.895863

24 H 9.572798 8.127942 10.447662 9.985831 7.836775

25 H 11.239032 9.829297 12.233835 11.426134 9.231711

26 H 10.216442 8.768249 11.174099 10.472359 8.046548

27 H 10.058066 8.709825 11.121821 10.104395 7.959501

6 7 8 9 10

6 S 0.000000

7 C 1.773444 0.000000

8 S 2.938778 1.793719 0.000000

9 S 3.068701 1.724593 3.072772 0.000000

10 C 4.418192 2.883164 1.826361 3.493441 0.000000

11 C 5.568123 4.067492 2.686535 4.508347 1.528958

12 C 6.940504 5.380103 4.116451 5.637663 2.575777

13 C 8.079603 6.589830 5.161946 6.861813 3.909438

14 H 2.451063 3.029131 4.286173 3.152365 5.711289

15 H 4.095230 5.726113 6.410738 6.716103 8.178800

16 H 3.016426 2.939035 2.990540 3.607774 4.578034

17 H 3.833094 4.335644 4.690951 4.818296 6.325989

18 H 3.133813 3.877600 3.855078 4.960632 5.652918

19 H 4.751133 3.421815 2.425450 4.219153 1.097837

20 H 4.497015 2.786843 2.407185 2.864340 1.091386

21 H 5.631318 4.080629 2.915949 4.221786 2.149161

22 H 5.651283 4.393439 2.723760 5.139204 2.155793

23 H 7.080994 5.618372 4.342287 6.060712 2.738704

24 H 7.228622 5.550156 4.584895 5.487251 2.907051

25 H 9.033259 7.518483 6.132131 7.740567 4.739077

26 H 8.271236 6.745712 5.411936 6.830433 4.307672

27 H 8.023727 6.694132 5.088781 7.205962 4.114723

11 12 13 14 15

11 C 0.000000

12 C 1.530979 0.000000

13 C 2.526348 1.532065 0.000000

14 H 6.543329 7.974210 8.953199 0.000000

15 H 9.009974 10.499849 11.355048 3.998582 0.000000

16 H 4.936293 6.453995 7.139479 2.515180 4.749725

17 H 6.686939 8.199343 8.814652 2.459400 3.878598

18 H 6.094844 7.619735 8.263034 3.080191 3.390740

19 H 2.191512 2.787065 4.168287 6.397375 8.529659

20 H 2.180778 2.960396 4.378897 5.551310 8.431383

21 H 1.098769 2.165553 2.832564 6.182021 8.940391

22 H 1.098859 2.141813 2.643707 6.724482 8.763271

23 H 2.151397 1.097182 2.154546 8.411274 10.694379

24 H 2.179885 1.098451 2.171425 8.110534 10.951888

25 H 3.489338 2.192017 1.095717 9.975042 12.388852

26 H 2.840608 2.184561 1.096884 8.844236 11.438607

27 H 2.724594 2.171746 1.096276 8.993533 11.051150

16 17 18 19 20

16 H 0.000000

17 H 1.765631 0.000000

18 H 1.778886 1.772698 0.000000

19 H 5.385358 7.103009 6.234457 0.000000

20 H 4.802100 6.491045 6.063193 1.782125 0.000000

21 H 4.527321 6.218154 5.900122 3.077762 2.439611

22 H 4.833493 6.539626 5.753154 2.600747 3.064767

23 H 6.982700 8.744821 7.985762 2.496442 3.233020

24 H 6.830822 8.557113 8.150331 3.191394 2.877579

25 H 8.220044 9.904094 9.334897 4.839064 5.135426

26 H 6.991387 8.591957 8.242082 4.797260 4.641871

27 H 6.996917 8.632317 7.930379 4.305461 4.805399

21 22 23 24 25

21 H 0.000000

22 H 1.759300 0.000000

23 H 3.060289 2.539111 0.000000

24 H 2.485197 3.062303 1.762273 0.000000

25 H 3.851750 3.648527 2.477790 2.557463 0.000000

26 H 2.708170 3.037417 3.075780 2.510162 1.768747

27 H 3.142153 2.376740 2.535322 3.080497 1.769878

26 27

26 H 0.000000

27 H 1.771789 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 4.52D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.076342 -0.389197 0.141333

2 6 0 -2.646949 -0.139099 0.557637

3 8 0 -5.021260 0.310044 0.445506

4 8 0 -4.232953 -1.595331 -0.462419

5 6 0 -2.033021 -1.326065 1.283705

6 16 0 -1.684187 0.338233 -1.026279

7 6 0 -0.098917 0.877183 -0.441852

8 16 0 1.097990 -0.456911 -0.512804

9 16 0 0.090369 2.207682 0.638964

10 6 0 2.722940 0.352171 -0.714098

11 6 0 3.702039 -0.445561 0.147703

12 6 0 5.177645 -0.111180 -0.086120

13 6 0 6.090884 -1.120653 0.616861

14 1 0 -2.646977 0.744866 1.190790

15 1 0 -5.177642 -1.761118 -0.627023

16 1 0 -0.990959 -1.118973 1.522213

17 1 0 -2.567584 -1.483474 2.228503

18 1 0 -2.094842 -2.245305 0.699259

19 1 0 3.007679 0.345835 -1.774348

20 1 0 2.640229 1.386186 -0.374842

21 1 0 3.448133 -0.288002 1.205059

22 1 0 3.563071 -1.517960 -0.047590

23 1 0 5.379354 -0.139087 -1.164241

24 1 0 5.407495 0.908044 0.252915

25 1 0 7.145728 -0.964560 0.364799

26 1 0 5.997639 -1.050712 1.707534

27 1 0 5.825955 -2.143090 0.323166

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2586834 0.1978461 0.1857165

Leave Link 202 at Sat Aug 17 17:43:49 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1103.1532640258 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0546198194 Hartrees.

Nuclear repulsion after empirical dispersion term = 1103.0986442065 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2330

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.32D-11

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 111

GePol: Fraction of low-weight points (<1% of avg) = 4.76%

GePol: Cavity surface area = 309.644 Ang\*\*2

GePol: Cavity volume = 320.342 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0049102250 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1103.0937339814 Hartrees.

Leave Link 301 at Sat Aug 17 17:43:50 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.96D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 296 296 296 296 296 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:43:50 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:43:50 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.996297 -0.085808 -0.004671 0.002792 Ang= -9.86 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.61906211174

Leave Link 401 at Sat Aug 17 17:43:50 2019, MaxMem= 1342177280 cpu: 7.6

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16286700.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.33D-15 for 577.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.93D-15 for 764 486.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.00D-15 for 2318.

Iteration 1 A^-1\*A deviation from orthogonality is 6.54D-13 for 807 751.

E= -1657.42895602282

DIIS: error= 3.40D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1657.42895602282 IErMin= 1 ErrMin= 3.40D-02

ErrMax= 3.40D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.67D+00 BMatP= 2.67D+00

IDIUse=3 WtCom= 6.60D-01 WtEn= 3.40D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Recover alternate guess density for next cycle.

RMSDP=4.19D-03 MaxDP=1.10D-01 OVMax= 0.00D+00

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.13D-03 CP: 9.58D-01

E= -1658.21884334183 Delta-E= -0.789887319015 Rises=F Damp=F

DIIS: error= 3.30D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.21884334183 IErMin= 2 ErrMin= 3.30D-02

ErrMax= 3.30D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.17D+00 BMatP= 2.67D+00

IDIUse=3 WtCom= 6.70D-01 WtEn= 3.30D-01

Coeff-Com: 0.441D+00 0.559D+00

Coeff-En: 0.000D+00 0.100D+01

Coeff: 0.295D+00 0.705D+00

Gap= 0.109 Goal= None Shift= 0.000

Gap= 0.144 Goal= None Shift= 0.000

RMSDP=3.75D-03 MaxDP=1.71D-01 DE=-7.90D-01 OVMax= 2.07D-01

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.31D-03 CP: 9.59D-01 5.74D-01

E= -1658.20576108582 Delta-E= 0.013082256010 Rises=F Damp=F

DIIS: error= 3.08D-02 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1658.21884334183 IErMin= 3 ErrMin= 3.08D-02

ErrMax= 3.08D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.14D+00 BMatP= 2.17D+00

IDIUse=3 WtCom= 6.92D-01 WtEn= 3.08D-01

Coeff-Com: 0.505D-01 0.469D+00 0.480D+00

Coeff-En: 0.000D+00 0.507D+00 0.493D+00

Coeff: 0.349D-01 0.481D+00 0.484D+00

Gap= 0.118 Goal= None Shift= 0.000

Gap= 0.129 Goal= None Shift= 0.000

RMSDP=2.16D-03 MaxDP=1.17D-01 DE= 1.31D-02 OVMax= 1.43D-01

Cycle 4 Pass 1 IDiag 1:

RMSU= 8.74D-04 CP: 9.57D-01 7.68D-01 4.55D-01

E= -1658.64071371045 Delta-E= -0.434952624630 Rises=F Damp=F

DIIS: error= 1.16D-02 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.64071371045 IErMin= 4 ErrMin= 1.16D-02

ErrMax= 1.16D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.50D-01 BMatP= 2.14D+00

IDIUse=3 WtCom= 8.84D-01 WtEn= 1.16D-01

Coeff-Com: -0.429D-02 0.216D+00 0.274D+00 0.514D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.379D-02 0.191D+00 0.242D+00 0.571D+00

Gap= 0.115 Goal= None Shift= 0.000

Gap= 0.130 Goal= None Shift= 0.000

RMSDP=6.58D-04 MaxDP=2.84D-02 DE=-4.35D-01 OVMax= 7.76D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.30D-04 CP: 9.59D-01 7.76D-01 5.04D-01 4.64D-01

E= -1658.65782746648 Delta-E= -0.017113756030 Rises=F Damp=F

DIIS: error= 8.79D-03 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.65782746648 IErMin= 5 ErrMin= 8.79D-03

ErrMax= 8.79D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.09D-02 BMatP= 1.50D-01

IDIUse=3 WtCom= 9.12D-01 WtEn= 8.79D-02

Coeff-Com: -0.406D-02 0.247D-01 0.561D-01 0.402D+00 0.521D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.327D+00 0.673D+00

Coeff: -0.370D-02 0.226D-01 0.511D-01 0.396D+00 0.534D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.130 Goal= None Shift= 0.000

RMSDP=3.17D-04 MaxDP=1.59D-02 DE=-1.71D-02 OVMax= 3.46D-02

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.62D-04 CP: 9.57D-01 7.70D-01 4.95D-01 6.68D-01 5.31D-01

E= -1658.66918133688 Delta-E= -0.011353870399 Rises=F Damp=F

DIIS: error= 1.65D-03 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.66918133688 IErMin= 6 ErrMin= 1.65D-03

ErrMax= 1.65D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.05D-03 BMatP= 6.09D-02

IDIUse=3 WtCom= 9.83D-01 WtEn= 1.65D-02

Coeff-Com: -0.883D-03 0.208D-02 0.127D-01 0.177D+00 0.286D+00 0.522D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.868D-03 0.204D-02 0.125D-01 0.174D+00 0.282D+00 0.530D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=6.64D-05 MaxDP=2.76D-03 DE=-1.14D-02 OVMax= 5.64D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 4.66D-05 CP: 9.57D-01 7.68D-01 4.96D-01 6.88D-01 6.06D-01

CP: 8.22D-01

E= -1658.66957348095 Delta-E= -0.000392144069 Rises=F Damp=F

DIIS: error= 3.81D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.66957348095 IErMin= 7 ErrMin= 3.81D-04

ErrMax= 3.81D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.54D-04 BMatP= 2.05D-03

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.81D-03

Coeff-Com: -0.251D-03-0.176D-02-0.738D-03 0.378D-01 0.744D-01 0.255D+00

Coeff-Com: 0.636D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00

Coeff-En: 0.100D+01

Coeff: -0.250D-03-0.175D-02-0.735D-03 0.377D-01 0.741D-01 0.254D+00

Coeff: 0.637D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=2.31D-05 MaxDP=8.50D-04 DE=-3.92D-04 OVMax= 2.19D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.92D-05 CP: 9.57D-01 7.68D-01 4.95D-01 6.96D-01 6.27D-01

CP: 8.53D-01 9.48D-01

E= -1658.66960884426 Delta-E= -0.000035363311 Rises=F Damp=F

DIIS: error= 9.42D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.66960884426 IErMin= 8 ErrMin= 9.42D-05

ErrMax= 9.42D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.20D-05 BMatP= 1.54D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.518D-05-0.116D-02-0.179D-02 0.263D-02 0.103D-01 0.741D-01

Coeff-Com: 0.303D+00 0.613D+00

Coeff: 0.518D-05-0.116D-02-0.179D-02 0.263D-02 0.103D-01 0.741D-01

Coeff: 0.303D+00 0.613D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=1.57D-05 MaxDP=5.61D-04 DE=-3.54D-05 OVMax= 2.26D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 8.42D-06 CP: 9.57D-01 7.68D-01 4.94D-01 7.00D-01 6.29D-01

CP: 9.14D-01 1.11D+00 9.89D-01

E= -1658.66961612687 Delta-E= -0.000007282611 Rises=F Damp=F

DIIS: error= 6.37D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.66961612687 IErMin= 9 ErrMin= 6.37D-05

ErrMax= 6.37D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.59D-06 BMatP= 2.20D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.881D-04-0.911D-04-0.784D-03-0.949D-02-0.160D-01-0.342D-01

Coeff-Com: -0.443D-01 0.265D+00 0.840D+00

Coeff: 0.881D-04-0.911D-04-0.784D-03-0.949D-02-0.160D-01-0.342D-01

Coeff: -0.443D-01 0.265D+00 0.840D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=9.08D-06 MaxDP=4.86D-04 DE=-7.28D-06 OVMax= 1.47D-03

Cycle 10 Pass 1 IDiag 1:

RMSU= 3.93D-06 CP: 9.57D-01 7.67D-01 4.94D-01 7.03D-01 6.35D-01

CP: 9.40D-01 1.19D+00 1.22D+00 9.16D-01

E= -1658.66961840744 Delta-E= -0.000002280574 Rises=F Damp=F

DIIS: error= 3.32D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.66961840744 IErMin=10 ErrMin= 3.32D-05

ErrMax= 3.32D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.33D-06 BMatP= 4.59D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.446D-04 0.220D-03-0.166D-03-0.764D-02-0.140D-01-0.412D-01

Coeff-Com: -0.981D-01 0.377D-01 0.565D+00 0.559D+00

Coeff: 0.446D-04 0.220D-03-0.166D-03-0.764D-02-0.140D-01-0.412D-01

Coeff: -0.981D-01 0.377D-01 0.565D+00 0.559D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=5.39D-06 MaxDP=2.78D-04 DE=-2.28D-06 OVMax= 8.35D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.72D-06 CP: 9.57D-01 7.67D-01 4.94D-01 7.05D-01 6.37D-01

CP: 9.54D-01 1.24D+00 1.33D+00 1.21D+00 7.91D-01

E= -1658.66961913099 Delta-E= -0.000000723549 Rises=F Damp=F

DIIS: error= 1.04D-05 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.66961913099 IErMin=11 ErrMin= 1.04D-05

ErrMax= 1.04D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.97D-07 BMatP= 2.33D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.161D-04 0.993D-04 0.425D-04-0.211D-02-0.386D-02-0.139D-01

Coeff-Com: -0.387D-01-0.252D-01 0.152D+00 0.265D+00 0.666D+00

Coeff: 0.161D-04 0.993D-04 0.425D-04-0.211D-02-0.386D-02-0.139D-01

Coeff: -0.387D-01-0.252D-01 0.152D+00 0.265D+00 0.666D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=1.16D-06 MaxDP=8.60D-05 DE=-7.24D-07 OVMax= 2.17D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 7.63D-07 CP: 9.57D-01 7.67D-01 4.94D-01 7.05D-01 6.37D-01

CP: 9.55D-01 1.24D+00 1.35D+00 1.23D+00 9.37D-01

CP: 8.39D-01

E= -1658.66961919423 Delta-E= -0.000000063234 Rises=F Damp=F

DIIS: error= 4.77D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.66961919423 IErMin=12 ErrMin= 4.77D-06

ErrMax= 4.77D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.68D-08 BMatP= 1.97D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.377D-05 0.975D-05 0.648D-04 0.408D-03 0.746D-03 0.497D-03

Coeff-Com: -0.105D-02-0.203D-01-0.311D-01 0.390D-02 0.353D+00 0.694D+00

Coeff: -0.377D-05 0.975D-05 0.648D-04 0.408D-03 0.746D-03 0.497D-03

Coeff: -0.105D-02-0.203D-01-0.311D-01 0.390D-02 0.353D+00 0.694D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=6.30D-07 MaxDP=3.46D-05 DE=-6.32D-08 OVMax= 6.40D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 3.06D-07 CP: 9.57D-01 7.67D-01 4.94D-01 7.05D-01 6.37D-01

CP: 9.56D-01 1.25D+00 1.35D+00 1.26D+00 9.72D-01

CP: 1.04D+00 9.40D-01

E= -1658.66961920971 Delta-E= -0.000000015486 Rises=F Damp=F

DIIS: error= 9.55D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1658.66961920971 IErMin=13 ErrMin= 9.55D-07

ErrMax= 9.55D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.88D-09 BMatP= 4.68D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.236D-05-0.921D-05 0.148D-04 0.406D-03 0.717D-03 0.196D-02

Coeff-Com: 0.492D-02-0.265D-02-0.279D-01-0.374D-01 0.411D-01 0.236D+00

Coeff-Com: 0.783D+00

Coeff: -0.236D-05-0.921D-05 0.148D-04 0.406D-03 0.717D-03 0.196D-02

Coeff: 0.492D-02-0.265D-02-0.279D-01-0.374D-01 0.411D-01 0.236D+00

Coeff: 0.783D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=1.99D-07 MaxDP=9.16D-06 DE=-1.55D-08 OVMax= 3.25D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 9.90D-08 CP: 9.57D-01 7.67D-01 4.94D-01 7.05D-01 6.37D-01

CP: 9.55D-01 1.25D+00 1.35D+00 1.26D+00 9.88D-01

CP: 1.09D+00 1.09D+00 9.53D-01

E= -1658.66961921100 Delta-E= -0.000000001289 Rises=F Damp=F

DIIS: error= 3.75D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1658.66961921100 IErMin=14 ErrMin= 3.75D-07

ErrMax= 3.75D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.59D-10 BMatP= 2.88D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.189D-06-0.246D-05-0.471D-05 0.597D-04 0.866D-04 0.505D-03

Coeff-Com: 0.148D-02 0.177D-02-0.311D-02-0.116D-01-0.368D-01-0.364D-01

Coeff-Com: 0.228D+00 0.856D+00

Coeff: -0.189D-06-0.246D-05-0.471D-05 0.597D-04 0.866D-04 0.505D-03

Coeff: 0.148D-02 0.177D-02-0.311D-02-0.116D-01-0.368D-01-0.364D-01

Coeff: 0.228D+00 0.856D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=8.81D-08 MaxDP=5.16D-06 DE=-1.29D-09 OVMax= 1.11D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 3.66D-08 CP: 9.57D-01 7.67D-01 4.94D-01 7.05D-01 6.37D-01

CP: 9.55D-01 1.25D+00 1.35D+00 1.26D+00 9.92D-01

CP: 1.11D+00 1.14D+00 1.12D+00 1.02D+00

E= -1658.66961921120 Delta-E= -0.000000000197 Rises=F Damp=F

DIIS: error= 1.95D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1658.66961921120 IErMin=15 ErrMin= 1.95D-07

ErrMax= 1.95D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.45D-11 BMatP= 3.59D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.102D-06-0.217D-06-0.407D-05-0.183D-04-0.436D-04 0.644D-05

Coeff-Com: 0.586D-04 0.982D-03 0.223D-02-0.737D-03-0.214D-01-0.465D-01

Coeff-Com: 0.179D-01 0.418D+00 0.629D+00

Coeff: 0.102D-06-0.217D-06-0.407D-05-0.183D-04-0.436D-04 0.644D-05

Coeff: 0.586D-04 0.982D-03 0.223D-02-0.737D-03-0.214D-01-0.465D-01

Coeff: 0.179D-01 0.418D+00 0.629D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=2.54D-08 MaxDP=1.33D-06 DE=-1.97D-10 OVMax= 4.49D-06

Cycle 16 Pass 1 IDiag 1:

RMSU= 1.48D-08 CP: 9.57D-01 7.67D-01 4.94D-01 7.05D-01 6.37D-01

CP: 9.55D-01 1.25D+00 1.35D+00 1.26D+00 9.94D-01

CP: 1.12D+00 1.15D+00 1.14D+00 1.14D+00 8.83D-01

E= -1658.66961921122 Delta-E= -0.000000000019 Rises=F Damp=F

DIIS: error= 5.52D-08 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1658.66961921122 IErMin=16 ErrMin= 5.52D-08

ErrMax= 5.52D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.90D-12 BMatP= 8.45D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.875D-07 0.128D-06-0.831D-06-0.132D-04-0.237D-04-0.515D-04

Coeff-Com: -0.137D-03 0.717D-04 0.106D-02 0.945D-03-0.279D-02-0.117D-01

Coeff-Com: -0.201D-01 0.346D-01 0.225D+00 0.774D+00

Coeff: 0.875D-07 0.128D-06-0.831D-06-0.132D-04-0.237D-04-0.515D-04

Coeff: -0.137D-03 0.717D-04 0.106D-02 0.945D-03-0.279D-02-0.117D-01

Coeff: -0.201D-01 0.346D-01 0.225D+00 0.774D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=9.55D-09 MaxDP=5.34D-07 DE=-1.91D-11 OVMax= 1.23D-06

Error on total polarization charges = 0.04157

SCF Done: E(UB3LYP) = -1658.66961921 A.U. after 16 cycles

NFock= 16 Conv=0.96D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655165869557D+03 PE=-6.148963621944D+03 EE= 1.732034399195D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.08

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:44:25 2019, MaxMem= 1342177280 cpu: 404.7

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 351

Leave Link 701 at Sat Aug 17 17:44:26 2019, MaxMem= 1342177280 cpu: 10.5

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:44:26 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:44:29 2019, MaxMem= 1342177280 cpu: 39.0

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.26661209D+00-3.28594893D+00 3.93409384D-03

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.009531907 -0.011055474 0.016927793

2 6 0.001032873 0.002220009 -0.010506477

3 8 0.006924443 -0.000012610 -0.009515224

4 8 0.002512097 0.005586083 -0.002870206

5 6 -0.002058977 0.000215031 0.001575183

6 16 -0.001269390 0.000496831 0.002777451

7 6 -0.004296705 -0.004135050 0.005219940

8 16 -0.006358331 -0.001481049 -0.005044365

9 16 -0.000311687 0.002538371 -0.001453576

10 6 0.004460698 -0.001811149 0.002588550

11 6 0.004158230 0.002370565 0.000632235

12 6 0.001108125 -0.002429126 -0.001644023

13 6 0.000589425 0.001905642 0.000753365

14 1 0.000415309 0.001501286 -0.001082086

15 1 0.000884237 0.004040479 0.001426902

16 1 0.001587419 0.000063719 0.000210748

17 1 0.000896702 -0.000908740 -0.000371200

18 1 0.001429515 0.001575754 -0.000219254

19 1 -0.000678852 -0.000738415 0.003461305

20 1 -0.000771434 -0.000323608 -0.000191860

21 1 0.000063301 -0.000864800 -0.002213040

22 1 0.000130999 0.001316114 0.000215792

23 1 0.000377778 0.000768124 0.000384444

24 1 -0.001338764 -0.001222542 -0.001001483

25 1 -0.000970653 0.000376441 0.000562537

26 1 -0.000151130 -0.000575745 -0.001338179

27 1 0.001166679 0.000583860 0.000714727

-------------------------------------------------------------------

Cartesian Forces: Max 0.016927793 RMS 0.003664033

Leave Link 716 at Sat Aug 17 17:44:29 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.017024378 RMS 0.003127577

Search for a local minimum.

Step number 32 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .31276D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

32 27

DE= 7.36D-03 DEPred=-4.47D-04 R=-1.64D+01

Trust test=-1.64D+01 RLast= 2.02D+00 DXMaxT set to 5.00D-02

ITU= -1 0 0 -1 -1 0 0 -1 0 0 -1 1 -1 1 -1 1 1 -1 1 -1

ITU= 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.97127.

Iteration 1 RMS(Cart)= 0.33480348 RMS(Int)= 0.11427966

Iteration 2 RMS(Cart)= 0.16284942 RMS(Int)= 0.06591858

Iteration 3 RMS(Cart)= 0.13738027 RMS(Int)= 0.03315903

Iteration 4 RMS(Cart)= 0.13171010 RMS(Int)= 0.00483261

Iteration 5 RMS(Cart)= 0.01028263 RMS(Int)= 0.00005026

Iteration 6 RMS(Cart)= 0.00004845 RMS(Int)= 0.00004675

Iteration 7 RMS(Cart)= 0.00000000 RMS(Int)= 0.00004675

ITry= 1 IFail=0 DXMaxC= 2.61D+00 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=T

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.85281 -0.00219 -0.01507 0.00000 -0.01507 2.83774

R2 2.29454 -0.00860 -0.00657 0.00000 -0.00657 2.28797

R3 2.56600 -0.00754 -0.01260 0.00000 -0.01260 2.55339

R4 2.87398 0.00037 -0.00717 0.00000 -0.00717 2.86681

R5 3.61701 -0.00671 -0.01955 0.00000 -0.01955 3.59745

R6 2.05475 0.00036 0.00312 0.00000 0.00312 2.05786

R7 1.83898 -0.00170 -0.00208 0.00000 -0.00208 1.83691

R8 2.05769 0.00158 0.00356 0.00000 0.00356 2.06125

R9 2.07283 -0.00050 -0.00403 0.00000 -0.00403 2.06880

R10 2.06180 -0.00117 -0.00151 0.00000 -0.00151 2.06028

R11 3.35132 -0.00293 -0.03015 0.00000 -0.03015 3.32118

R12 3.38964 0.00311 -0.00536 0.00000 -0.00536 3.38428

R13 3.25901 0.00064 -0.00487 0.00000 -0.00487 3.25414

R14 3.45132 0.00670 0.02412 0.00000 0.02412 3.47544

R15 2.88931 0.00070 -0.00817 0.00000 -0.00817 2.88115

R16 2.07461 -0.00358 -0.01064 0.00000 -0.01064 2.06397

R17 2.06242 -0.00033 -0.00218 0.00000 -0.00218 2.06024

R18 2.89313 0.00082 0.00106 0.00000 0.00106 2.89419

R19 2.07637 -0.00219 -0.00398 0.00000 -0.00398 2.07240

R20 2.07654 -0.00132 -0.00554 0.00000 -0.00554 2.07101

R21 2.89518 -0.00098 -0.00907 0.00000 -0.00907 2.88611

R22 2.07337 -0.00024 -0.00139 0.00000 -0.00139 2.07198

R23 2.07577 -0.00179 -0.00399 0.00000 -0.00399 2.07178

R24 2.07060 -0.00100 -0.00291 0.00000 -0.00291 2.06770

R25 2.07281 -0.00127 -0.00357 0.00000 -0.00357 2.06924

R26 2.07166 -0.00109 -0.00263 0.00000 -0.00263 2.06903

A1 2.18017 0.00056 -0.00275 0.00000 -0.00260 2.17757

A2 1.95948 0.00204 0.01578 0.00000 0.01593 1.97541

A3 2.13312 -0.00144 -0.00348 0.00000 -0.00334 2.12979

A4 1.96554 0.00397 0.05611 0.00000 0.05612 2.02166

A5 1.86437 -0.00050 -0.02580 0.00000 -0.02581 1.83856

A6 1.87050 -0.00173 0.00102 0.00000 0.00105 1.87155

A7 1.96780 -0.00197 -0.02087 0.00000 -0.02088 1.94692

A8 1.93532 0.00003 0.00462 0.00000 0.00465 1.93997

A9 1.85370 -0.00003 -0.02107 0.00000 -0.02106 1.83263

A10 1.91611 -0.00713 -0.04174 0.00000 -0.04174 1.87438

A11 1.92033 -0.00020 -0.00848 0.00000 -0.00848 1.91184

A12 1.90338 0.00219 0.02457 0.00000 0.02457 1.92795

A13 1.95946 -0.00100 -0.00695 0.00000 -0.00695 1.95251

A14 1.88075 -0.00062 0.00289 0.00000 0.00289 1.88364

A15 1.90900 -0.00032 -0.01525 0.00000 -0.01525 1.89376

A16 1.88901 -0.00003 0.00350 0.00000 0.00350 1.89251

A17 1.82628 -0.00691 -0.03242 0.00000 -0.03242 1.79386

A18 1.93629 0.00393 0.03449 0.00000 0.03474 1.97103

A19 2.14016 -0.00260 0.00179 0.00000 0.00205 2.14221

A20 2.12392 0.00193 0.02942 0.00000 0.02967 2.15359

A21 1.84270 -0.00808 -0.04817 0.00000 -0.04817 1.79453

A22 1.85094 0.01702 0.07537 0.00000 0.07537 1.92631

A23 1.91203 -0.00493 -0.03631 0.00000 -0.03632 1.87571

A24 1.89444 -0.00667 0.00064 0.00000 0.00066 1.89510

A25 1.95547 -0.00480 -0.01632 0.00000 -0.01633 1.93914

A26 1.94727 -0.00239 -0.00861 0.00000 -0.00859 1.93868

A27 1.90216 0.00176 -0.01518 0.00000 -0.01517 1.88699

A28 2.00112 -0.00437 -0.04732 0.00000 -0.04732 1.95381

A29 1.89612 0.00086 0.02121 0.00000 0.02123 1.91735

A30 1.90501 0.00167 0.01002 0.00000 0.01002 1.91503

A31 1.91599 0.00129 -0.00968 0.00000 -0.00968 1.90631

A32 1.88378 0.00163 0.02567 0.00000 0.02567 1.90945

A33 1.85641 -0.00084 0.00307 0.00000 0.00307 1.85948

A34 1.93964 0.00451 0.02684 0.00000 0.02685 1.96649

A35 1.89833 -0.00037 0.00790 0.00000 0.00792 1.90625

A36 1.93606 -0.00265 -0.02840 0.00000 -0.02841 1.90766

A37 1.90131 -0.00070 0.01121 0.00000 0.01123 1.91254

A38 1.92306 -0.00135 -0.01007 0.00000 -0.01008 1.91298

A39 1.86337 0.00042 -0.00883 0.00000 -0.00883 1.85454

A40 1.95458 -0.00074 -0.00905 0.00000 -0.00905 1.94553

A41 1.94288 0.00028 -0.00053 0.00000 -0.00052 1.94236

A42 1.92574 0.00148 0.01744 0.00000 0.01744 1.94318

A43 1.87706 0.00003 -0.00060 0.00000 -0.00060 1.87646

A44 1.87956 -0.00029 -0.00251 0.00000 -0.00251 1.87705

A45 1.88106 -0.00081 -0.00522 0.00000 -0.00522 1.87584

D1 2.16518 0.00459 0.48697 0.00000 0.48696 2.65214

D2 -1.94855 0.00432 0.47786 0.00000 0.47786 -1.47068

D3 0.03228 0.00325 0.44267 0.00000 0.44267 0.47496

D4 -0.82418 -0.00371 0.30427 0.00000 0.30427 -0.51991

D5 1.34528 -0.00398 0.29516 0.00000 0.29516 1.64044

D6 -2.95708 -0.00505 0.25997 0.00000 0.25998 -2.69710

D7 3.03395 0.00507 0.14187 0.00000 0.14187 -3.10737

D8 0.03987 -0.00317 -0.03516 0.00000 -0.03516 0.00471

D9 3.09506 -0.00011 0.06698 0.00000 0.06698 -3.12115

D10 -1.12876 0.00033 0.08021 0.00000 0.08022 -1.04854

D11 0.96463 0.00113 0.09681 0.00000 0.09682 1.06145

D12 0.98373 -0.00092 0.07555 0.00000 0.07555 1.05928

D13 3.04309 -0.00049 0.08879 0.00000 0.08879 3.13188

D14 -1.14670 0.00032 0.10539 0.00000 0.10539 -1.04131

D15 -1.09224 0.00041 0.11259 0.00000 0.11259 -0.97965

D16 0.96713 0.00084 0.12583 0.00000 0.12582 1.09295

D17 3.06053 0.00165 0.14243 0.00000 0.14242 -3.08023

D18 2.98263 -0.00173 0.14925 0.00000 0.14925 3.13188

D19 -1.13248 0.00165 0.18818 0.00000 0.18818 -0.94430

D20 0.99039 0.00049 0.16838 0.00000 0.16838 1.15877

D21 1.67342 0.00560 0.16808 0.00000 0.16809 1.84151

D22 -1.04749 -0.00288 -0.06507 0.00000 -0.06508 -1.11257

D23 2.66078 -0.00241 -0.10724 0.00000 -0.10719 2.55359

D24 -0.89696 0.00471 0.12008 0.00000 0.12003 -0.77693

D25 2.45988 0.00143 0.80591 0.00000 0.80590 -3.01741

D26 -1.70971 0.00300 0.80936 0.00000 0.80937 -0.90034

D27 0.36547 -0.00167 0.77143 0.00000 0.77144 1.13691

D28 2.94042 0.00113 0.23264 0.00000 0.23264 -3.11013

D29 -1.19228 0.00040 0.20320 0.00000 0.20321 -0.98907

D30 0.82509 0.00077 0.22453 0.00000 0.22453 1.04963

D31 0.85507 -0.00088 0.23906 0.00000 0.23905 1.09412

D32 3.00555 -0.00162 0.20962 0.00000 0.20963 -3.06801

D33 -1.26026 -0.00125 0.23095 0.00000 0.23095 -1.02931

D34 -1.28315 0.00207 0.27598 0.00000 0.27597 -1.00718

D35 0.86733 0.00133 0.24654 0.00000 0.24654 1.11388

D36 2.88471 0.00170 0.26787 0.00000 0.26787 -3.13061

D37 -2.95968 -0.00169 -0.16339 0.00000 -0.16339 -3.12307

D38 -0.86667 -0.00002 -0.12668 0.00000 -0.12669 -0.99336

D39 1.17770 -0.00127 -0.14885 0.00000 -0.14886 1.02884

D40 1.18373 -0.00067 -0.15101 0.00000 -0.15100 1.03272

D41 -3.00645 0.00100 -0.11431 0.00000 -0.11430 -3.12075

D42 -0.96208 -0.00025 -0.13647 0.00000 -0.13647 -1.09855

D43 -0.83274 -0.00125 -0.16369 0.00000 -0.16369 -0.99643

D44 1.26027 0.00042 -0.12699 0.00000 -0.12699 1.13328

D45 -2.97855 -0.00083 -0.14915 0.00000 -0.14915 -3.12771

D46 3.02610 0.00148 0.11463 0.00000 0.11463 3.14072

D47 -1.15503 0.00120 0.10732 0.00000 0.10732 -1.04771

D48 0.93265 0.00133 0.11202 0.00000 0.11201 1.04467

D49 0.93486 -0.00040 0.07971 0.00000 0.07971 1.01457

D50 3.03692 -0.00067 0.07239 0.00000 0.07240 3.10931

D51 -1.15859 -0.00054 0.07709 0.00000 0.07710 -1.08149

D52 -1.10381 0.00027 0.08962 0.00000 0.08962 -1.01419

D53 0.99825 -0.00001 0.08231 0.00000 0.08231 1.08055

D54 3.08593 0.00013 0.08701 0.00000 0.08701 -3.11025

Item Value Threshold Converged?

Maximum Force 0.017024 0.000450 NO

RMS Force 0.003128 0.000300 NO

Maximum Displacement 2.609653 0.001800 NO

RMS Displacement 0.674880 0.001200 NO

Predicted change in Energy=-3.534875D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:44:30 2019, MaxMem= 1342177280 cpu: 0.6

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.108439 -0.369949 -0.210841

2 6 0 -2.836844 0.055617 0.465138

3 8 0 -4.898391 0.384271 -0.733358

4 8 0 -4.284006 -1.709669 -0.218799

5 6 0 -2.342989 -0.851912 1.575965

6 16 0 -1.552738 0.214055 -0.931289

7 6 0 -0.106978 0.726894 -0.073648

8 16 0 1.104823 -0.580853 0.095475

9 16 0 -0.003697 2.228620 0.762706

10 6 0 2.701209 0.327642 0.002939

11 6 0 3.867739 -0.652837 -0.045933

12 6 0 5.219274 0.066795 -0.078958

13 6 0 6.399251 -0.899916 -0.154195

14 1 0 -2.987800 1.071941 0.825920

15 1 0 -5.108799 -1.891796 -0.699865

16 1 0 -1.430435 -0.437876 2.006772

17 1 0 -3.090024 -0.922492 2.373122

18 1 0 -2.129227 -1.857791 1.213793

19 1 0 2.672755 0.950031 -0.894131

20 1 0 2.777562 0.985001 0.869341

21 1 0 3.833276 -1.316537 0.826414

22 1 0 3.775049 -1.294171 -0.929765

23 1 0 5.245496 0.746262 -0.939093

24 1 0 5.316206 0.696880 0.812983

25 1 0 7.353834 -0.365641 -0.177649

26 1 0 6.418707 -1.571548 0.710410

27 1 0 6.347345 -1.522660 -1.053232

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.501668 0.000000

3 O 1.210742 2.407152 0.000000

4 O 1.351198 2.382915 2.242058 0.000000

5 C 2.557690 1.517050 3.659399 2.779293 0.000000

6 S 2.718771 1.903691 3.355823 3.415872 2.836743

7 C 4.151334 2.862353 4.848736 4.837919 3.195871

8 S 5.226511 4.009798 6.136531 5.514750 3.762012

9 S 4.954721 3.582905 5.440392 5.898688 3.952639

10 C 6.848624 5.563961 7.635396 7.279631 5.413843

11 C 7.982896 6.761252 8.853992 8.221783 6.422097

12 C 9.338864 8.074479 10.143776 9.668905 7.795552

13 C 10.521199 9.306023 11.385134 10.714096 8.911932

14 H 2.099941 1.088975 2.560195 3.241750 2.163229

15 H 1.885705 3.211141 2.286017 0.972049 3.729674

16 H 3.477661 2.144332 4.495660 3.835817 1.090768

17 H 2.831843 2.158982 3.824662 2.960286 1.094761

18 H 2.856666 2.173095 4.060359 2.591782 1.090255

19 H 6.942177 5.744846 7.593957 7.478408 5.874186

20 H 7.100682 5.705145 7.864462 7.636166 5.485764

21 H 8.064909 6.819371 9.031481 8.193734 6.238906

22 H 7.969970 6.890922 8.836532 8.101016 6.626059

23 H 9.448406 8.232440 10.152429 9.867209 8.152594

24 H 9.539930 8.185624 10.335709 9.950885 7.851380

25 H 11.462322 10.219616 12.287726 11.715264 9.866104

26 H 10.635476 9.400694 11.575250 10.743862 8.833708

27 H 10.552809 9.441701 11.410753 10.665686 9.104092

6 7 8 9 10

6 S 0.000000

7 C 1.757490 0.000000

8 S 2.957829 1.790885 0.000000

9 S 3.054115 1.722015 3.093082 0.000000

10 C 4.356805 2.837461 1.839124 3.392268 0.000000

11 C 5.560299 4.207470 2.767468 4.893332 1.524637

12 C 6.827027 5.367004 4.168763 5.715007 2.532864

13 C 8.067152 6.707013 5.309906 7.185136 3.899629

14 H 2.425522 3.037665 4.473795 3.201058 5.796215

15 H 4.139292 5.680483 6.400019 6.721533 8.149605

16 H 3.012006 2.726971 3.178212 3.270089 4.655304

17 H 3.817607 4.195917 4.785513 4.695569 6.381144

18 H 3.037477 3.525278 3.652435 4.628187 5.438327

19 H 4.289269 2.906871 2.404441 3.397542 1.092205

20 H 4.752696 3.045721 2.418434 3.048501 1.090231

21 H 5.868678 4.528943 2.918896 5.224419 2.159401

22 H 5.537152 4.459571 2.947888 5.436307 2.157161

23 H 6.819038 5.422025 4.469534 5.713801 2.745189

24 H 7.103379 5.495266 4.459054 5.536255 2.762375

25 H 8.957178 7.541099 6.258678 7.857971 4.707459

26 H 8.332316 6.962913 5.440311 7.462659 4.234056

27 H 8.089645 6.904952 5.448905 7.596411 4.222963

11 12 13 14 15

11 C 0.000000

12 C 1.531538 0.000000

13 C 2.545844 1.527265 0.000000

14 H 7.122738 8.317763 9.641865 0.000000

15 H 9.085201 10.530466 11.563598 3.950999 0.000000

16 H 5.685988 6.987389 8.135554 2.469685 4.792716

17 H 7.371229 8.719853 9.820091 2.526271 3.802400

18 H 6.245192 7.705563 8.690446 3.077487 3.541341

19 H 2.171776 2.815915 4.225706 5.917374 8.286513

20 H 2.169959 2.775668 4.209177 5.766180 8.540085

21 H 1.096666 2.157382 2.778380 7.227164 9.089618

22 H 1.095929 2.159141 2.764667 7.376790 8.906894

23 H 2.157180 1.096447 2.158036 8.426654 10.687750

24 H 2.158131 1.096340 2.158281 8.312481 10.847612

25 H 3.500384 2.180157 1.094179 10.489193 12.566586

26 H 2.814876 2.178511 1.094993 9.771579 11.617867

27 H 2.814194 2.179019 1.094884 9.869554 11.467535

16 17 18 19 20

16 H 0.000000

17 H 1.767287 0.000000

18 H 1.770109 1.772558 0.000000

19 H 5.213223 6.884106 5.948633 0.000000

20 H 4.585364 6.350469 5.681257 1.766930 0.000000

21 H 5.465523 7.104904 5.999538 3.073177 2.532479

22 H 6.037678 7.627348 6.306582 2.500553 3.070242

23 H 7.392453 9.123399 8.111877 2.581190 3.068897

24 H 6.944780 8.701788 7.881717 3.156922 2.555563

25 H 9.052088 10.765254 9.700055 4.914961 4.884945

26 H 8.035845 9.674806 8.567526 4.792189 4.451870

27 H 8.428181 10.058034 8.780887 4.431944 4.767389

21 22 23 24 25

21 H 0.000000

22 H 1.757286 0.000000

23 H 3.060478 2.515089 0.000000

24 H 2.500622 3.062127 1.754197 0.000000

25 H 3.782417 3.773003 2.502242 2.502445 0.000000

26 H 2.600566 3.123467 3.077260 2.524242 1.765594

27 H 3.145806 2.585374 2.524898 3.077721 1.765887

26 27

26 H 0.000000

27 H 1.765761 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 6.40D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.118643 -0.424193 -0.150391

2 6 0 -2.841812 0.105374 0.436354

3 8 0 -4.912901 0.234682 -0.783585

4 8 0 -4.293954 -1.746792 0.063464

5 6 0 -2.338928 -0.607657 1.677376

6 16 0 -1.568888 0.030629 -0.977193

7 6 0 -0.116474 0.675966 -0.226988

8 16 0 1.096939 -0.587469 0.145338

9 16 0 -0.006896 2.294673 0.350175

10 6 0 2.692327 0.291720 -0.107923

11 6 0 3.858660 -0.684703 -0.004079

12 6 0 5.209722 0.018244 -0.165651

13 6 0 6.389289 -0.948949 -0.090183

14 1 0 -2.990132 1.167353 0.626266

15 1 0 -5.122505 -2.004662 -0.374585

16 1 0 -1.423074 -0.129395 2.027022

17 1 0 -3.079585 -0.545379 2.481150

18 1 0 -2.127817 -1.659630 1.483881

19 1 0 2.656594 0.758143 -1.094880

20 1 0 2.775413 1.082526 0.637950

21 1 0 3.831290 -1.195873 0.965783

22 1 0 3.759094 -1.462552 -0.769650

23 1 0 5.228944 0.546983 -1.125996

24 1 0 5.313596 0.786325 0.609734

25 1 0 7.343530 -0.426834 -0.208705

26 1 0 6.415777 -1.469274 0.872921

27 1 0 6.330381 -1.711005 -0.874130

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3284120 0.1920229 0.1799243

Leave Link 202 at Sat Aug 17 17:44:30 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1101.4385324095 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0549110669 Hartrees.

Nuclear repulsion after empirical dispersion term = 1101.3836213426 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2322

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.19D-08

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 102

GePol: Fraction of low-weight points (<1% of avg) = 4.39%

GePol: Cavity surface area = 309.736 Ang\*\*2

GePol: Cavity volume = 320.357 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057712769 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1101.3778500657 Hartrees.

Leave Link 301 at Sat Aug 17 17:44:30 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:44:30 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:44:30 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Lowest energy guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999996 -0.002869 -0.000194 -0.000105 Ang= -0.33 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.996566 0.082632 0.004492 -0.002926 Ang= 9.50 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 2.87D-02

Max alpha theta= 27.499 degrees.

Max beta theta= 27.850 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 17:44:30 2019, MaxMem= 1342177280 cpu: 4.3

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16175052.

Iteration 1 A\*A^-1 deviation from unit magnitude is 4.00D-15 for 2312.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.83D-15 for 2310 1782.

Iteration 1 A^-1\*A deviation from unit magnitude is 4.22D-15 for 2308.

Iteration 1 A^-1\*A deviation from orthogonality is 9.13D-12 for 794 763.

E= -1658.67682501287

DIIS: error= 8.91D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67682501287 IErMin= 1 ErrMin= 8.91D-04

ErrMax= 8.91D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.41D-04 BMatP= 6.41D-04

IDIUse=3 WtCom= 9.91D-01 WtEn= 8.91D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 88.705 Goal= None Shift= 0.000

Gap= 88.705 Goal= None Shift= 0.000

RMSDP=5.22D-05 MaxDP=3.14D-03 OVMax= 4.42D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 5.20D-05 CP: 1.00D+00

E= -1658.67681190561 Delta-E= 0.000013107256 Rises=F Damp=F

DIIS: error= 9.44D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 1 EnMin= -1658.67682501287 IErMin= 1 ErrMin= 8.91D-04

ErrMax= 9.44D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.38D-04 BMatP= 6.41D-04

IDIUse=3 WtCom= 2.46D-01 WtEn= 7.54D-01

Coeff-Com: 0.557D+00 0.443D+00

Coeff-En: 0.526D+00 0.474D+00

Coeff: 0.534D+00 0.466D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.26D-05 MaxDP=2.68D-03 DE= 1.31D-05 OVMax= 3.62D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.89D-05 CP: 1.00D+00 4.01D-01

E= -1658.67695371043 Delta-E= -0.000141804821 Rises=F Damp=F

DIIS: error= 4.44D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67695371043 IErMin= 3 ErrMin= 4.44D-04

ErrMax= 4.44D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.50D-04 BMatP= 6.41D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 4.44D-03

Coeff-Com: 0.574D-01 0.284D+00 0.659D+00

Coeff-En: 0.000D+00 0.161D+00 0.839D+00

Coeff: 0.572D-01 0.283D+00 0.660D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.57D-05 MaxDP=7.94D-04 DE=-1.42D-04 OVMax= 1.67D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 8.74D-06 CP: 1.00D+00 5.73D-01 6.72D-01

E= -1658.67697565986 Delta-E= -0.000021949425 Rises=F Damp=F

DIIS: error= 2.36D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67697565986 IErMin= 4 ErrMin= 2.36D-04

ErrMax= 2.36D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.57D-05 BMatP= 1.50D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.36D-03

Coeff-Com: -0.125D-01 0.147D+00 0.433D+00 0.432D+00

Coeff-En: 0.000D+00 0.000D+00 0.106D+00 0.894D+00

Coeff: -0.125D-01 0.147D+00 0.432D+00 0.433D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.42D-06 MaxDP=2.82D-04 DE=-2.19D-05 OVMax= 5.46D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.83D-06 CP: 1.00D+00 5.68D-01 7.48D-01 4.75D-01

E= -1658.67698021928 Delta-E= -0.000004559422 Rises=F Damp=F

DIIS: error= 2.49D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67698021928 IErMin= 5 ErrMin= 2.49D-05

ErrMax= 2.49D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.09D-07 BMatP= 2.57D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.905D-02 0.571D-01 0.176D+00 0.211D+00 0.566D+00

Coeff: -0.905D-02 0.571D-01 0.176D+00 0.211D+00 0.566D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=9.20D-07 MaxDP=5.85D-05 DE=-4.56D-06 OVMax= 6.50D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 6.80D-07 CP: 1.00D+00 5.70D-01 7.52D-01 4.88D-01 6.77D-01

E= -1658.67698030114 Delta-E= -0.000000081865 Rises=F Damp=F

DIIS: error= 4.35D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67698030114 IErMin= 6 ErrMin= 4.35D-06

ErrMax= 4.35D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.03D-08 BMatP= 5.09D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.285D-02 0.140D-01 0.447D-01 0.601D-01 0.255D+00 0.629D+00

Coeff: -0.285D-02 0.140D-01 0.447D-01 0.601D-01 0.255D+00 0.629D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.99D-07 MaxDP=1.70D-05 DE=-8.19D-08 OVMax= 2.87D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.10D-07 CP: 1.00D+00 5.70D-01 7.51D-01 4.95D-01 7.38D-01

CP: 7.58D-01

E= -1658.67698030738 Delta-E= -0.000000006235 Rises=F Damp=F

DIIS: error= 1.52D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67698030738 IErMin= 7 ErrMin= 1.52D-06

ErrMax= 1.52D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.18D-09 BMatP= 3.03D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.488D-03 0.160D-02 0.558D-02 0.889D-02 0.614D-01 0.267D+00

Coeff-Com: 0.656D+00

Coeff: -0.488D-03 0.160D-02 0.558D-02 0.889D-02 0.614D-01 0.267D+00

Coeff: 0.656D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.20D-07 MaxDP=5.52D-06 DE=-6.24D-09 OVMax= 1.37D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 8.52D-08 CP: 1.00D+00 5.70D-01 7.52D-01 4.96D-01 7.45D-01

CP: 8.19D-01 7.11D-01

E= -1658.67698030791 Delta-E= -0.000000000534 Rises=F Damp=F

DIIS: error= 5.47D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67698030791 IErMin= 8 ErrMin= 5.47D-07

ErrMax= 5.47D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.57D-10 BMatP= 2.18D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.512D-04-0.693D-03-0.204D-02-0.216D-02 0.225D-02 0.648D-01

Coeff-Com: 0.339D+00 0.599D+00

Coeff: 0.512D-04-0.693D-03-0.204D-02-0.216D-02 0.225D-02 0.648D-01

Coeff: 0.339D+00 0.599D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.84D-08 MaxDP=1.61D-06 DE=-5.34D-10 OVMax= 3.49D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.21D-08 CP: 1.00D+00 5.70D-01 7.52D-01 4.96D-01 7.49D-01

CP: 8.30D-01 8.11D-01 7.69D-01

E= -1658.67698030798 Delta-E= -0.000000000071 Rises=F Damp=F

DIIS: error= 5.88D-08 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67698030798 IErMin= 9 ErrMin= 5.88D-08

ErrMax= 5.88D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.08D-11 BMatP= 3.57D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.523D-04-0.372D-03-0.115D-02-0.144D-02-0.383D-02 0.357D-02

Coeff-Com: 0.668D-01 0.186D+00 0.750D+00

Coeff: 0.523D-04-0.372D-03-0.115D-02-0.144D-02-0.383D-02 0.357D-02

Coeff: 0.668D-01 0.186D+00 0.750D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.20D-08 MaxDP=6.61D-07 DE=-7.09D-11 OVMax= 1.72D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 7.91D-09 CP: 1.00D+00 5.70D-01 7.52D-01 4.96D-01 7.50D-01

CP: 8.33D-01 8.30D-01 8.53D-01 1.05D+00

E= -1658.67698030802 Delta-E= -0.000000000034 Rises=F Damp=F

DIIS: error= 3.23D-08 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67698030802 IErMin=10 ErrMin= 3.23D-08

ErrMax= 3.23D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.23D-12 BMatP= 1.08D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.127D-04-0.416D-04-0.142D-03-0.236D-03-0.176D-02-0.712D-02

Coeff-Com: -0.213D-01-0.126D-01 0.285D+00 0.758D+00

Coeff: 0.127D-04-0.416D-04-0.142D-03-0.236D-03-0.176D-02-0.712D-02

Coeff: -0.213D-01-0.126D-01 0.285D+00 0.758D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.29D-09 MaxDP=4.41D-07 DE=-3.37D-11 OVMax= 1.12D-06

Error on total polarization charges = 0.04170

SCF Done: E(UB3LYP) = -1658.67698031 A.U. after 10 cycles

NFock= 10 Conv=0.63D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655236125618D+03 PE=-6.145518013422D+03 EE= 1.730227057431D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.62

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:44:53 2019, MaxMem= 1342177280 cpu: 257.6

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 338

Leave Link 701 at Sat Aug 17 17:44:54 2019, MaxMem= 1342177280 cpu: 10.3

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:44:54 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:44:57 2019, MaxMem= 1342177280 cpu: 38.5

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.36985664D+00-2.92996335D+00 5.74124569D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000047605 -0.000143209 0.000359491

2 6 -0.000188628 -0.000422726 0.000184436

3 8 -0.000173728 0.000161998 -0.000312547

4 8 0.000174892 -0.000019861 -0.000034320

5 6 0.000143688 0.000010450 -0.000017799

6 16 0.000127062 0.000393747 -0.000091610

7 6 -0.000216326 0.000009660 0.000011027

8 16 0.000285073 -0.000163887 0.000123311

9 16 -0.000106790 -0.000029785 0.000049912

10 6 -0.000193238 0.000022116 0.000014376

11 6 0.000009222 -0.000091996 -0.000037555

12 6 -0.000084780 0.000074546 -0.000115513

13 6 0.000044616 -0.000105008 0.000040871

14 1 0.000010737 0.000080245 -0.000081893

15 1 -0.000029542 0.000129320 -0.000025529

16 1 0.000147911 -0.000037143 0.000075804

17 1 0.000006749 0.000010372 0.000013416

18 1 -0.000013951 0.000010782 -0.000070164

19 1 0.000158046 0.000132092 -0.000024418

20 1 -0.000126217 -0.000110023 0.000102938

21 1 -0.000047233 0.000046942 -0.000019502

22 1 0.000052939 -0.000032141 -0.000058711

23 1 -0.000000757 0.000046225 0.000023925

24 1 0.000009314 -0.000042127 0.000031036

25 1 -0.000003845 0.000016352 -0.000005087

26 1 -0.000001461 -0.000029457 -0.000051697

27 1 -0.000031357 0.000082520 -0.000084198

-------------------------------------------------------------------

Cartesian Forces: Max 0.000422726 RMS 0.000123988

Leave Link 716 at Sat Aug 17 17:44:57 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000774220 RMS 0.000132528

Search for a local minimum.

Step number 33 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .13253D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 1 3 4 5 6

2 8 9 10 11

12 13 14 15 16

17 18 20 21 22

23 24 19 26 28

30 31 27 33

ITU= 0 -1 0 0 -1 -1 0 0 -1 0 0 -1 1 -1 1 -1 1 1 -1 1

ITU= -1 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Use linear search instead of GDIIS.

Eigenvalues --- 0.00011 0.00092 0.00148 0.00259 0.00392

Eigenvalues --- 0.00412 0.00736 0.00901 0.01409 0.01856

Eigenvalues --- 0.02334 0.03155 0.03366 0.03592 0.04396

Eigenvalues --- 0.04527 0.04808 0.04845 0.05369 0.05416

Eigenvalues --- 0.05478 0.05529 0.05656 0.05831 0.07967

Eigenvalues --- 0.08229 0.08340 0.11010 0.11893 0.12111

Eigenvalues --- 0.13305 0.13651 0.15277 0.15738 0.16006

Eigenvalues --- 0.16010 0.16123 0.16330 0.16637 0.17052

Eigenvalues --- 0.19214 0.19754 0.21565 0.21912 0.22813

Eigenvalues --- 0.24262 0.24700 0.25071 0.25487 0.26417

Eigenvalues --- 0.27144 0.27508 0.28433 0.29287 0.29592

Eigenvalues --- 0.30017 0.30496 0.30883 0.32510 0.33714

Eigenvalues --- 0.33881 0.33885 0.33940 0.33971 0.34038

Eigenvalues --- 0.34073 0.34095 0.34254 0.34341 0.34550

Eigenvalues --- 0.34729 0.35718 0.49688 0.53360 0.79164

RFO step: Lambda=-4.68531370D-05 EMin= 1.10034849D-04

Quartic linear search produced a step of -0.28656.

Iteration 1 RMS(Cart)= 0.03660618 RMS(Int)= 0.00035814

Iteration 2 RMS(Cart)= 0.00087968 RMS(Int)= 0.00000971

Iteration 3 RMS(Cart)= 0.00000037 RMS(Int)= 0.00000971

ITry= 1 IFail=0 DXMaxC= 1.23D-01 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83774 -0.00004 -0.00013 0.00336 0.00323 2.84097

R2 2.28797 0.00034 -0.00006 0.00403 0.00397 2.29194

R3 2.55339 -0.00009 -0.00011 0.00296 0.00285 2.55624

R4 2.86681 0.00003 -0.00006 0.00009 0.00003 2.86684

R5 3.59745 0.00000 -0.00017 0.00428 0.00412 3.60157

R6 2.05786 0.00005 0.00003 0.00132 0.00135 2.05921

R7 1.83691 0.00000 -0.00002 0.00159 0.00157 1.83847

R8 2.06125 0.00015 0.00003 0.00073 0.00076 2.06202

R9 2.06880 0.00001 -0.00003 0.00086 0.00082 2.06962

R10 2.06028 -0.00003 -0.00001 0.00159 0.00158 2.06186

R11 3.32118 -0.00027 -0.00026 -0.00070 -0.00096 3.32022

R12 3.38428 0.00023 -0.00005 -0.00020 -0.00025 3.38403

R13 3.25414 -0.00003 -0.00004 0.00127 0.00123 3.25537

R14 3.47544 -0.00021 0.00020 0.00153 0.00174 3.47718

R15 2.88115 0.00003 -0.00007 0.00137 0.00130 2.88244

R16 2.06397 0.00010 -0.00009 0.00116 0.00107 2.06503

R17 2.06024 -0.00001 -0.00002 0.00161 0.00159 2.06183

R18 2.89419 -0.00006 0.00001 0.00141 0.00142 2.89561

R19 2.07240 -0.00003 -0.00003 0.00112 0.00109 2.07349

R20 2.07101 0.00005 -0.00005 0.00108 0.00104 2.07204

R21 2.88611 0.00005 -0.00008 0.00150 0.00142 2.88754

R22 2.07198 0.00001 -0.00001 0.00108 0.00106 2.07305

R23 2.07178 0.00000 -0.00003 0.00109 0.00105 2.07284

R24 2.06770 0.00000 -0.00002 0.00127 0.00124 2.06894

R25 2.06924 0.00000 -0.00003 0.00105 0.00102 2.07026

R26 2.06903 0.00001 -0.00002 0.00127 0.00124 2.07028

A1 2.17757 0.00016 -0.00007 -0.00114 -0.00124 2.17633

A2 1.97541 -0.00014 0.00009 0.00154 0.00159 1.97700

A3 2.12979 -0.00003 -0.00007 -0.00080 -0.00091 2.12888

A4 2.02166 0.00018 0.00047 0.00261 0.00308 2.02474

A5 1.83856 0.00000 -0.00022 -0.00269 -0.00290 1.83565

A6 1.87155 -0.00001 0.00000 0.00268 0.00268 1.87423

A7 1.94692 -0.00012 -0.00017 -0.00453 -0.00471 1.94221

A8 1.93997 -0.00002 0.00003 -0.00227 -0.00225 1.93773

A9 1.83263 -0.00005 -0.00018 0.00466 0.00448 1.83711

A10 1.87438 -0.00019 -0.00035 0.00389 0.00354 1.87791

A11 1.91184 0.00008 -0.00007 -0.00326 -0.00334 1.90851

A12 1.92795 -0.00004 0.00021 0.00000 0.00021 1.92816

A13 1.95251 -0.00007 -0.00006 0.00140 0.00134 1.95385

A14 1.88364 -0.00002 0.00002 0.00130 0.00132 1.88496

A15 1.89376 -0.00001 -0.00013 0.00019 0.00006 1.89381

A16 1.89251 0.00006 0.00003 0.00043 0.00046 1.89297

A17 1.79386 -0.00077 -0.00027 0.00046 0.00019 1.79405

A18 1.97103 -0.00032 0.00022 -0.00148 -0.00130 1.96973

A19 2.14221 -0.00003 -0.00006 0.00012 0.00001 2.14222

A20 2.15359 0.00030 0.00018 -0.00212 -0.00199 2.15160

A21 1.79453 0.00031 -0.00041 0.00127 0.00086 1.79539

A22 1.92631 -0.00028 0.00064 0.00072 0.00136 1.92767

A23 1.87571 0.00026 -0.00031 -0.00059 -0.00090 1.87481

A24 1.89510 -0.00006 0.00000 0.00042 0.00041 1.89552

A25 1.93914 -0.00008 -0.00014 0.00039 0.00025 1.93939

A26 1.93868 0.00017 -0.00008 -0.00121 -0.00129 1.93739

A27 1.88699 0.00000 -0.00013 0.00030 0.00017 1.88715

A28 1.95381 0.00007 -0.00040 0.00062 0.00022 1.95403

A29 1.91735 -0.00007 0.00017 0.00030 0.00048 1.91782

A30 1.91503 0.00003 0.00009 -0.00002 0.00007 1.91510

A31 1.90631 0.00001 -0.00008 -0.00089 -0.00097 1.90534

A32 1.90945 -0.00006 0.00022 -0.00030 -0.00008 1.90937

A33 1.85948 0.00002 0.00002 0.00025 0.00028 1.85976

A34 1.96649 -0.00010 0.00023 0.00030 0.00053 1.96702

A35 1.90625 0.00006 0.00006 0.00103 0.00110 1.90735

A36 1.90766 0.00001 -0.00024 -0.00143 -0.00167 1.90598

A37 1.91254 0.00002 0.00009 0.00059 0.00068 1.91322

A38 1.91298 0.00004 -0.00008 -0.00050 -0.00058 1.91240

A39 1.85454 -0.00001 -0.00007 -0.00001 -0.00009 1.85446

A40 1.94553 0.00000 -0.00008 0.00045 0.00037 1.94590

A41 1.94236 0.00003 0.00000 -0.00039 -0.00039 1.94197

A42 1.94318 -0.00009 0.00015 -0.00055 -0.00040 1.94278

A43 1.87646 0.00000 -0.00001 0.00055 0.00054 1.87700

A44 1.87705 0.00003 -0.00002 -0.00033 -0.00035 1.87670

A45 1.87584 0.00003 -0.00004 0.00030 0.00026 1.87610

D1 2.65214 0.00014 0.00413 0.04571 0.04984 2.70198

D2 -1.47068 0.00010 0.00405 0.03951 0.04356 -1.42712

D3 0.47496 0.00005 0.00375 0.04469 0.04844 0.52339

D4 -0.51991 0.00001 0.00258 0.03109 0.03367 -0.48624

D5 1.64044 -0.00003 0.00250 0.02489 0.02739 1.66784

D6 -2.69710 -0.00008 0.00220 0.03007 0.03227 -2.66483

D7 -3.10737 0.00004 0.00120 0.01056 0.01176 -3.09561

D8 0.00471 -0.00008 -0.00030 -0.00362 -0.00392 0.00079

D9 -3.12115 -0.00004 0.00057 -0.01029 -0.00972 -3.13087

D10 -1.04854 -0.00004 0.00068 -0.01072 -0.01004 -1.05858

D11 1.06145 -0.00004 0.00082 -0.00923 -0.00841 1.05304

D12 1.05928 -0.00008 0.00064 -0.00504 -0.00439 1.05488

D13 3.13188 -0.00008 0.00075 -0.00547 -0.00471 3.12717

D14 -1.04131 -0.00008 0.00089 -0.00398 -0.00308 -1.04439

D15 -0.97965 0.00007 0.00096 -0.00653 -0.00558 -0.98522

D16 1.09295 0.00007 0.00107 -0.00696 -0.00589 1.08706

D17 -3.08023 0.00007 0.00121 -0.00547 -0.00426 -3.08450

D18 3.13188 0.00026 0.00127 0.03493 0.03618 -3.11512

D19 -0.94430 0.00041 0.00159 0.03345 0.03506 -0.90924

D20 1.15877 0.00028 0.00143 0.03112 0.03254 1.19131

D21 1.84151 -0.00017 0.00142 -0.02535 -0.02393 1.81758

D22 -1.11257 0.00008 -0.00055 -0.00539 -0.00594 -1.11850

D23 2.55359 0.00025 -0.00092 0.01236 0.01143 2.56502

D24 -0.77693 -0.00005 0.00103 -0.00747 -0.00643 -0.78335

D25 -3.01741 0.00011 0.00684 -0.02496 -0.01812 -3.03553

D26 -0.90034 0.00001 0.00686 -0.02443 -0.01757 -0.91791

D27 1.13691 0.00012 0.00654 -0.02418 -0.01764 1.11927

D28 -3.11013 0.00007 0.00197 0.00385 0.00583 -3.10430

D29 -0.98907 0.00008 0.00172 0.00336 0.00508 -0.98399

D30 1.04963 0.00008 0.00190 0.00383 0.00573 1.05536

D31 1.09412 -0.00002 0.00203 0.00388 0.00591 1.10003

D32 -3.06801 -0.00001 0.00178 0.00338 0.00516 -3.06285

D33 -1.02931 -0.00001 0.00196 0.00385 0.00581 -1.02350

D34 -1.00718 -0.00008 0.00234 0.00406 0.00640 -1.00078

D35 1.11388 -0.00007 0.00209 0.00356 0.00565 1.11953

D36 -3.13061 -0.00007 0.00227 0.00403 0.00630 -3.12431

D37 -3.12307 -0.00001 -0.00138 0.01272 0.01134 -3.11173

D38 -0.99336 -0.00002 -0.00107 0.01442 0.01334 -0.98001

D39 1.02884 0.00001 -0.00126 0.01418 0.01292 1.04176

D40 1.03272 0.00002 -0.00128 0.01254 0.01126 1.04398

D41 -3.12075 0.00002 -0.00097 0.01423 0.01326 -3.10749

D42 -1.09855 0.00004 -0.00116 0.01400 0.01284 -1.08572

D43 -0.99643 0.00003 -0.00139 0.01291 0.01152 -0.98491

D44 1.13328 0.00002 -0.00108 0.01460 0.01352 1.14680

D45 -3.12771 0.00005 -0.00126 0.01436 0.01310 -3.11461

D46 3.14072 0.00001 0.00097 0.00890 0.00987 -3.13259

D47 -1.04771 0.00003 0.00091 0.00964 0.01055 -1.03717

D48 1.04467 0.00004 0.00095 0.00939 0.01034 1.05500

D49 1.01457 0.00000 0.00067 0.00695 0.00763 1.02219

D50 3.10931 0.00002 0.00061 0.00769 0.00830 3.11762

D51 -1.08149 0.00002 0.00065 0.00744 0.00809 -1.07340

D52 -1.01419 -0.00002 0.00076 0.00692 0.00768 -1.00652

D53 1.08055 0.00000 0.00070 0.00765 0.00835 1.08890

D54 -3.11025 0.00001 0.00074 0.00740 0.00814 -3.10211

Item Value Threshold Converged?

Maximum Force 0.000774 0.000450 NO

RMS Force 0.000133 0.000300 YES

Maximum Displacement 0.122593 0.001800 NO

RMS Displacement 0.036731 0.001200 NO

Predicted change in Energy=-2.685818D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:44:57 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.102865 -0.391415 -0.202321

2 6 0 -2.838351 0.067654 0.468802

3 8 0 -4.897813 0.341234 -0.752114

4 8 0 -4.256955 -1.735260 -0.190068

5 6 0 -2.301684 -0.833911 1.564545

6 16 0 -1.571745 0.272797 -0.940441

7 6 0 -0.116400 0.763409 -0.087059

8 16 0 1.083258 -0.558075 0.058894

9 16 0 -0.002960 2.243762 0.786588

10 6 0 2.689452 0.336683 -0.013923

11 6 0 3.849412 -0.653018 -0.053872

12 6 0 5.207671 0.056194 -0.062050

13 6 0 6.381466 -0.918650 -0.144035

14 1 0 -3.016008 1.075297 0.843652

15 1 0 -5.072571 -1.942243 -0.678354

16 1 0 -1.393965 -0.394944 1.981692

17 1 0 -3.033455 -0.930843 2.373600

18 1 0 -2.064353 -1.831598 1.192019

19 1 0 2.674913 0.962605 -0.909554

20 1 0 2.763281 0.990822 0.856187

21 1 0 3.798157 -1.323231 0.813381

22 1 0 3.764334 -1.287190 -0.944294

23 1 0 5.247551 0.752763 -0.908592

24 1 0 5.300706 0.668028 0.843592

25 1 0 7.341315 -0.392024 -0.139427

26 1 0 6.381516 -1.612709 0.703593

27 1 0 6.338254 -1.517775 -1.060220

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.503378 0.000000

3 O 1.212844 2.409743 0.000000

4 O 1.352706 2.386849 2.244643 0.000000

5 C 2.561614 1.517064 3.672568 2.777442 0.000000

6 S 2.718927 1.905870 3.332098 3.435943 2.834178

7 C 4.151964 2.863926 4.845868 4.837164 3.170913

8 S 5.195371 3.992315 6.102433 5.474086 3.714957

9 S 4.973059 3.588297 5.472367 5.906179 3.919365

10 C 6.833827 5.555359 7.623092 7.250969 5.364074

11 C 7.957963 6.746757 8.831196 8.179425 6.363016

12 C 9.322344 8.063523 10.133027 9.633527 7.734889

13 C 10.497741 9.292653 11.365703 10.669817 8.850058

14 H 2.103940 1.089687 2.574200 3.241568 2.162180

15 H 1.889974 3.216736 2.291342 0.972879 3.733203

16 H 3.479664 2.142215 4.504731 3.835323 1.091173

17 H 2.840772 2.159472 3.855398 2.952361 1.095197

18 H 2.858993 2.174690 4.065630 2.593637 1.091091

19 H 6.947793 5.752989 7.599807 7.473081 5.840818

20 H 7.083430 5.690395 7.854996 7.603282 5.430036

21 H 8.020354 6.789444 8.991169 8.127824 6.165367

22 H 7.952720 6.886792 8.815979 8.069121 6.579994

23 H 9.446599 8.230942 10.154912 9.850998 8.100919

24 H 9.520688 8.169772 10.327771 9.909245 7.782797

25 H 11.444353 10.208176 12.276372 11.675904 9.802358

26 H 10.594078 9.374684 11.539507 10.676644 8.760464

27 H 10.536681 9.437244 11.392982 10.633105 9.055694

6 7 8 9 10

6 S 0.000000

7 C 1.756983 0.000000

8 S 2.956021 1.790754 0.000000

9 S 3.054246 1.722665 3.091876 0.000000

10 C 4.361229 2.839058 1.840042 3.395121 0.000000

11 C 5.570645 4.211298 2.770079 4.892696 1.525324

12 C 6.839515 5.370894 4.171659 5.714570 2.534248

13 C 8.081298 6.712290 5.314340 7.185249 3.901764

14 H 2.431643 3.061246 4.481934 3.232186 5.816636

15 H 4.151008 5.677482 6.352454 6.735699 8.116894

16 H 3.002723 2.693267 3.140127 3.213400 4.603483

17 H 3.816833 4.175469 4.737525 4.666972 6.329183

18 H 3.036203 3.487782 3.579565 4.585005 5.362313

19 H 4.302429 2.916780 2.404938 3.418957 1.092769

20 H 4.747198 3.038749 2.420173 3.037564 1.091072

21 H 5.870183 4.526435 2.919828 5.212739 2.160781

22 H 5.559435 4.472125 2.954009 5.445740 2.158223

23 H 6.836240 5.426509 4.471651 5.715293 2.741792

24 H 7.111228 5.497295 4.461608 5.533088 2.768351

25 H 8.973643 7.546873 6.263401 7.857688 4.710265

26 H 8.337406 6.963762 5.440536 7.459275 4.236307

27 H 8.111016 6.914723 5.457877 7.600714 4.224631

11 12 13 14 15

11 C 0.000000

12 C 1.532291 0.000000

13 C 2.547546 1.528018 0.000000

14 H 7.136289 8.335932 9.657322 0.000000

15 H 9.036252 10.490803 11.512089 3.956198 0.000000

16 H 5.630553 6.925460 8.077767 2.467340 4.796052

17 H 7.303675 8.650017 9.745737 2.523023 3.807275

18 H 6.157427 7.617006 8.599440 3.078481 3.543997

19 H 2.172988 2.820408 4.226544 5.955923 8.277385

20 H 2.170276 2.773396 4.211625 5.779920 8.506366

21 H 1.097242 2.157759 2.784567 7.224037 9.016555

22 H 1.096478 2.160152 2.761452 7.399401 8.865140

23 H 2.159065 1.097010 2.159614 8.453449 10.668691

24 H 2.157976 1.096898 2.158934 8.326680 10.804383

25 H 3.502689 2.181588 1.094836 10.506837 12.521908

26 H 2.811816 2.179303 1.095532 9.775400 11.541857

27 H 2.820439 2.179894 1.095543 9.891965 11.425100

16 17 18 19 20

16 H 0.000000

17 H 1.768815 0.000000

18 H 1.771151 1.773881 0.000000

19 H 5.172815 6.851986 5.889382 0.000000

20 H 4.524357 6.292654 5.602222 1.768175 0.000000

21 H 5.402296 7.018489 5.896680 3.074935 2.535279

22 H 5.997128 7.572671 6.231678 2.499925 3.071347

23 H 7.333533 9.065450 8.034639 2.581182 3.056585

24 H 6.873413 8.622967 7.785475 3.170975 2.557905

25 H 8.989120 10.688382 9.607899 4.919698 4.884865

26 H 7.973368 9.586217 8.462811 4.793056 4.460188

27 H 8.384580 9.998227 8.704876 4.426630 4.769287

21 22 23 24 25

21 H 0.000000

22 H 1.758370 0.000000

23 H 3.061974 2.522422 0.000000

24 H 2.494730 3.062654 1.755037 0.000000

25 H 3.785361 3.774113 2.507191 2.500825 0.000000

26 H 2.601844 3.109845 3.079038 2.527748 1.766909

27 H 3.162328 2.586827 2.523483 3.078756 1.766722

26 27

26 H 0.000000

27 H 1.766895 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 4.76D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.108895 -0.452792 -0.130519

2 6 0 -2.838850 0.111001 0.443300

3 8 0 -4.908823 0.178110 -0.788598

4 8 0 -4.262342 -1.775387 0.108249

5 6 0 -2.292440 -0.594594 1.670107

6 16 0 -1.584467 0.075570 -0.991137

7 6 0 -0.122046 0.700825 -0.244565

8 16 0 1.079345 -0.578723 0.110710

9 16 0 -0.001698 2.306608 0.367439

10 6 0 2.684500 0.289467 -0.124829

11 6 0 3.844466 -0.694133 -0.008121

12 6 0 5.202324 0.002238 -0.146708

13 6 0 6.375759 -0.973779 -0.074048

14 1 0 -3.013682 1.167423 0.645351

15 1 0 -5.082036 -2.060472 -0.331434

16 1 0 -1.381348 -0.092839 1.999970

17 1 0 -3.017202 -0.553702 2.490170

18 1 0 -2.057919 -1.640874 1.468169

19 1 0 2.662026 0.756335 -1.112591

20 1 0 2.765535 1.080186 0.622589

21 1 0 3.800923 -1.209356 0.959654

22 1 0 3.752001 -1.468563 -0.778817

23 1 0 5.234660 0.546928 -1.098390

24 1 0 5.302886 0.757191 0.642670

25 1 0 7.335403 -0.454846 -0.166011

26 1 0 6.383359 -1.515855 0.877943

27 1 0 6.324922 -1.718023 -0.876375

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3102008 0.1930759 0.1806208

Leave Link 202 at Sat Aug 17 17:44:57 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.0255338231 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0550108746 Hartrees.

Nuclear repulsion after empirical dispersion term = 1101.9705229484 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2315

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.19D-08

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 96

GePol: Fraction of low-weight points (<1% of avg) = 4.15%

GePol: Cavity surface area = 309.418 Ang\*\*2

GePol: Cavity volume = 320.577 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057341009 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1101.9647888475 Hartrees.

Leave Link 301 at Sat Aug 17 17:44:57 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.86D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:44:57 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:44:57 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000360 -0.000663 -0.000229 Ang= -0.09 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.62902617026

Leave Link 401 at Sat Aug 17 17:44:58 2019, MaxMem= 1342177280 cpu: 7.6

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16077675.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.22D-15 for 182.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.92D-15 for 2252 2052.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.00D-15 for 183.

Iteration 1 A^-1\*A deviation from orthogonality is 3.67D-10 for 941 915.

Iteration 2 A\*A^-1 deviation from unit magnitude is 9.44D-15 for 1348.

Iteration 2 A\*A^-1 deviation from orthogonality is 5.52D-15 for 1623 1148.

Iteration 2 A^-1\*A deviation from unit magnitude is 9.99D-16 for 182.

Iteration 2 A^-1\*A deviation from orthogonality is 5.29D-16 for 2308 2129.

E= -1658.67450334013

DIIS: error= 1.53D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67450334013 IErMin= 1 ErrMin= 1.53D-03

ErrMax= 1.53D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.73D-03 BMatP= 5.73D-03

IDIUse=3 WtCom= 9.85D-01 WtEn= 1.53D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.429 Goal= None Shift= 0.000

Gap= 0.483 Goal= None Shift= 0.000

GapD= 0.429 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=1.77D-04 MaxDP=4.36D-03 OVMax= 9.76D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.77D-04 CP: 1.00D+00

E= -1658.67691260281 Delta-E= -0.002409262682 Rises=F Damp=F

DIIS: error= 1.87D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67691260281 IErMin= 2 ErrMin= 1.87D-04

ErrMax= 1.87D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.87D-05 BMatP= 5.73D-03

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.87D-03

Coeff-Com: -0.567D-01 0.106D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.566D-01 0.106D+01

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=2.82D-05 MaxDP=7.13D-04 DE=-2.41D-03 OVMax= 2.49D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.64D-05 CP: 1.00D+00 1.06D+00

E= -1658.67693431539 Delta-E= -0.000021712584 Rises=F Damp=F

DIIS: error= 1.87D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67693431539 IErMin= 2 ErrMin= 1.87D-04

ErrMax= 1.87D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.73D-05 BMatP= 9.87D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.87D-03

Coeff-Com: -0.333D-01 0.478D+00 0.556D+00

Coeff-En: 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.332D-01 0.477D+00 0.556D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=1.30D-05 MaxDP=6.29D-04 DE=-2.17D-05 OVMax= 7.41D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 9.06D-06 CP: 1.00D+00 1.08D+00 6.84D-01

E= -1658.67694378645 Delta-E= -0.000009471056 Rises=F Damp=F

DIIS: error= 1.16D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67694378645 IErMin= 4 ErrMin= 1.16D-04

ErrMax= 1.16D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.14D-05 BMatP= 5.73D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.16D-03

Coeff-Com: -0.115D-01 0.152D+00 0.327D+00 0.532D+00

Coeff-En: 0.000D+00 0.000D+00 0.126D+00 0.874D+00

Coeff: -0.115D-01 0.152D+00 0.327D+00 0.533D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=5.21D-06 MaxDP=2.20D-04 DE=-9.47D-06 OVMax= 4.93D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.28D-06 CP: 1.00D+00 1.08D+00 7.46D-01 7.49D-01

E= -1658.67694581200 Delta-E= -0.000002025550 Rises=F Damp=F

DIIS: error= 3.66D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67694581200 IErMin= 5 ErrMin= 3.66D-05

ErrMax= 3.66D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.21D-07 BMatP= 1.14D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.352D-02 0.419D-01 0.137D+00 0.298D+00 0.527D+00

Coeff: -0.352D-02 0.419D-01 0.137D+00 0.298D+00 0.527D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=1.65D-06 MaxDP=6.51D-05 DE=-2.03D-06 OVMax= 1.57D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.30D-06 CP: 1.00D+00 1.09D+00 7.62D-01 8.21D-01 8.43D-01

E= -1658.67694598666 Delta-E= -0.000000174665 Rises=F Damp=F

DIIS: error= 1.26D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67694598666 IErMin= 6 ErrMin= 1.26D-05

ErrMax= 1.26D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.79D-07 BMatP= 9.21D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.422D-03-0.101D-01 0.112D-01 0.682D-01 0.329D+00 0.601D+00

Coeff: 0.422D-03-0.101D-01 0.112D-01 0.682D-01 0.329D+00 0.601D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=9.58D-07 MaxDP=4.91D-05 DE=-1.75D-07 OVMax= 1.29D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 6.16D-07 CP: 1.00D+00 1.09D+00 7.81D-01 8.46D-01 9.43D-01

CP: 8.30D-01

E= -1658.67694602755 Delta-E= -0.000000040882 Rises=F Damp=F

DIIS: error= 3.74D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67694602755 IErMin= 7 ErrMin= 3.74D-06

ErrMax= 3.74D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.74D-08 BMatP= 1.79D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.675D-03-0.109D-01-0.125D-01-0.542D-02 0.913D-01 0.294D+00

Coeff-Com: 0.643D+00

Coeff: 0.675D-03-0.109D-01-0.125D-01-0.542D-02 0.913D-01 0.294D+00

Coeff: 0.643D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=3.83D-07 MaxDP=1.60D-05 DE=-4.09D-08 OVMax= 4.20D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.70D-07 CP: 1.00D+00 1.09D+00 7.84D-01 8.60D-01 9.84D-01

CP: 9.14D-01 1.08D+00

E= -1658.67694603312 Delta-E= -0.000000005572 Rises=F Damp=F

DIIS: error= 1.16D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67694603312 IErMin= 8 ErrMin= 1.16D-06

ErrMax= 1.16D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.71D-09 BMatP= 1.74D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.181D-03-0.212D-02-0.725D-02-0.154D-01-0.257D-01 0.561D-05

Coeff-Com: 0.272D+00 0.778D+00

Coeff: 0.181D-03-0.212D-02-0.725D-02-0.154D-01-0.257D-01 0.561D-05

Coeff: 0.272D+00 0.778D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=2.40D-07 MaxDP=8.70D-06 DE=-5.57D-09 OVMax= 3.38D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.01D-07 CP: 1.00D+00 1.09D+00 7.86D-01 8.67D-01 1.01D+00

CP: 9.86D-01 1.30D+00 9.92D-01

E= -1658.67694603441 Delta-E= -0.000000001291 Rises=F Damp=F

DIIS: error= 7.05D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67694603441 IErMin= 9 ErrMin= 7.05D-07

ErrMax= 7.05D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.83D-10 BMatP= 2.71D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.294D-04 0.103D-02-0.172D-02-0.785D-02-0.325D-01-0.589D-01

Coeff-Com: 0.184D-01 0.429D+00 0.653D+00

Coeff: -0.294D-04 0.103D-02-0.172D-02-0.785D-02-0.325D-01-0.589D-01

Coeff: 0.184D-01 0.429D+00 0.653D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=1.17D-07 MaxDP=4.46D-06 DE=-1.29D-09 OVMax= 1.68D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 4.65D-08 CP: 1.00D+00 1.09D+00 7.88D-01 8.69D-01 1.02D+00

CP: 9.99D-01 1.40D+00 1.20D+00 8.27D-01

E= -1658.67694603470 Delta-E= -0.000000000295 Rises=F Damp=F

DIIS: error= 4.44D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67694603470 IErMin=10 ErrMin= 4.44D-07

ErrMax= 4.44D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.08D-10 BMatP= 8.83D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.495D-04 0.984D-03 0.153D-03-0.220D-02-0.146D-01-0.359D-01

Coeff-Com: -0.443D-01 0.113D+00 0.390D+00 0.593D+00

Coeff: -0.495D-04 0.984D-03 0.153D-03-0.220D-02-0.146D-01-0.359D-01

Coeff: -0.443D-01 0.113D+00 0.390D+00 0.593D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=3.85D-08 MaxDP=2.24D-06 DE=-2.95D-10 OVMax= 5.83D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 2.31D-08 CP: 1.00D+00 1.09D+00 7.88D-01 8.70D-01 1.02D+00

CP: 1.01D+00 1.42D+00 1.24D+00 9.32D-01 7.52D-01

E= -1658.67694603476 Delta-E= -0.000000000053 Rises=F Damp=F

DIIS: error= 1.68D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67694603476 IErMin=11 ErrMin= 1.68D-07

ErrMax= 1.68D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.97D-11 BMatP= 2.08D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.210D-04 0.343D-03 0.327D-03 0.385D-04-0.215D-02-0.930D-02

Coeff-Com: -0.261D-01-0.688D-02 0.947D-01 0.352D+00 0.597D+00

Coeff: -0.210D-04 0.343D-03 0.327D-03 0.385D-04-0.215D-02-0.930D-02

Coeff: -0.261D-01-0.688D-02 0.947D-01 0.352D+00 0.597D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=1.91D-08 MaxDP=7.99D-07 DE=-5.32D-11 OVMax= 2.49D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 9.17D-09 CP: 1.00D+00 1.09D+00 7.88D-01 8.69D-01 1.02D+00

CP: 1.01D+00 1.43D+00 1.26D+00 9.88D-01 9.30D-01

CP: 7.96D-01

E= -1658.67694603482 Delta-E= -0.000000000062 Rises=F Damp=F

DIIS: error= 6.92D-08 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.67694603482 IErMin=12 ErrMin= 6.92D-08

ErrMax= 6.92D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.98D-12 BMatP= 3.97D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.140D-05-0.674D-04 0.116D-03 0.525D-03 0.258D-02 0.406D-02

Coeff-Com: -0.200D-02-0.296D-01-0.531D-01 0.320D-01 0.257D+00 0.789D+00

Coeff: 0.140D-05-0.674D-04 0.116D-03 0.525D-03 0.258D-02 0.406D-02

Coeff: -0.200D-02-0.296D-01-0.531D-01 0.320D-01 0.257D+00 0.789D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=6.66D-09 MaxDP=3.47D-07 DE=-6.18D-11 OVMax= 7.70D-07

Error on total polarization charges = 0.04167

SCF Done: E(UB3LYP) = -1658.67694603 A.U. after 12 cycles

NFock= 12 Conv=0.67D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655204681301D+03 PE=-6.146671266097D+03 EE= 1.730824849913D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.60

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:45:25 2019, MaxMem= 1342177280 cpu: 311.2

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 337

Leave Link 701 at Sat Aug 17 17:45:26 2019, MaxMem= 1342177280 cpu: 10.3

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:45:26 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:45:29 2019, MaxMem= 1342177280 cpu: 38.8

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.40507500D+00-2.95487222D+00 5.97878881D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000602770 0.000544698 -0.002552736

2 6 -0.001331523 -0.001106985 0.000578793

3 8 0.001524562 -0.001573173 0.001886946

4 8 -0.000050180 0.001008697 0.000363574

5 6 0.000059306 -0.000249379 0.000206504

6 16 -0.000018394 0.000766311 -0.000101960

7 6 -0.000317424 0.000074635 0.000612331

8 16 0.001133564 -0.000230985 -0.000038119

9 16 -0.000107439 -0.000113185 -0.000534725

10 6 -0.000095600 0.000300457 0.000199766

11 6 0.000032758 -0.000291540 -0.000265862

12 6 -0.000076019 0.000271996 0.000122003

13 6 -0.000004202 -0.000087450 -0.000154172

14 1 0.000015877 -0.000209013 -0.000538146

15 1 0.000615963 0.000807932 0.000326605

16 1 -0.000245270 -0.000361329 0.000207157

17 1 0.000278445 0.000080991 -0.000228840

18 1 -0.000249727 0.000561085 0.000047779

19 1 0.000291515 -0.000013310 0.000296995

20 1 -0.000346937 -0.000452363 -0.000274231

21 1 -0.000105707 0.000284500 -0.000361750

22 1 0.000045333 0.000134855 0.000213937

23 1 0.000002957 -0.000272546 0.000250745

24 1 -0.000003433 -0.000158596 -0.000299686

25 1 -0.000431429 -0.000144243 -0.000013638

26 1 0.000026062 0.000212236 -0.000296815

27 1 -0.000040290 0.000215704 0.000347546

-------------------------------------------------------------------

Cartesian Forces: Max 0.002552736 RMS 0.000578718

Leave Link 716 at Sat Aug 17 17:45:29 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.002807035 RMS 0.000451823

Search for a local minimum.

Step number 34 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .45182D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 33 34

DE= 3.43D-05 DEPred=-2.69D-05 R=-1.28D+00

Trust test=-1.28D+00 RLast= 1.35D-01 DXMaxT set to 5.00D-02

ITU= -1 0 -1 0 0 -1 -1 0 0 -1 0 0 -1 1 -1 1 -1 1 1 -1

ITU= 1 -1 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Eigenvalues --- 0.00028 0.00113 0.00187 0.00273 0.00298

Eigenvalues --- 0.00411 0.00565 0.00684 0.01464 0.02169

Eigenvalues --- 0.02357 0.03531 0.03619 0.04293 0.04572

Eigenvalues --- 0.04771 0.04839 0.04986 0.05117 0.05433

Eigenvalues --- 0.05477 0.05523 0.05644 0.05854 0.08058

Eigenvalues --- 0.08249 0.08351 0.10966 0.11667 0.12174

Eigenvalues --- 0.13286 0.14081 0.15525 0.15959 0.15999

Eigenvalues --- 0.16054 0.16136 0.16266 0.16824 0.17378

Eigenvalues --- 0.19458 0.19929 0.21899 0.22213 0.23063

Eigenvalues --- 0.24484 0.25016 0.25357 0.25752 0.26475

Eigenvalues --- 0.27540 0.27686 0.29067 0.29311 0.29624

Eigenvalues --- 0.30183 0.31469 0.32647 0.33672 0.33831

Eigenvalues --- 0.33882 0.33895 0.33952 0.34036 0.34045

Eigenvalues --- 0.34085 0.34174 0.34314 0.34561 0.34634

Eigenvalues --- 0.34870 0.35853 0.52548 0.55398 0.92544

En-DIIS/RFO-DIIS IScMMF= 0 using points: 34 33

RFO step: Lambda=-5.06399586D-05.

NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=F DC= -3.43D-05 SmlDif= 1.00D-05

RMS Error= 0.1281804093D-02 NUsed= 2 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.31740 0.68260

Iteration 1 RMS(Cart)= 0.10538753 RMS(Int)= 0.00299142

Iteration 2 RMS(Cart)= 0.00693879 RMS(Int)= 0.00002613

Iteration 3 RMS(Cart)= 0.00002146 RMS(Int)= 0.00002511

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00002511

ITry= 1 IFail=0 DXMaxC= 3.21D-01 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.84097 -0.00149 -0.00221 -0.00461 -0.00682 2.83415

R2 2.29194 -0.00281 -0.00271 -0.00564 -0.00835 2.28359

R3 2.55624 -0.00183 -0.00194 -0.00330 -0.00525 2.55100

R4 2.86684 0.00003 -0.00002 -0.00077 -0.00079 2.86605

R5 3.60157 0.00025 -0.00281 0.01725 0.01444 3.61601

R6 2.05921 -0.00038 -0.00092 -0.00192 -0.00284 2.05637

R7 1.83847 -0.00086 -0.00107 -0.00289 -0.00396 1.83452

R8 2.06202 -0.00026 -0.00052 -0.00078 -0.00130 2.06071

R9 2.06962 -0.00036 -0.00056 -0.00163 -0.00219 2.06743

R10 2.06186 -0.00061 -0.00108 -0.00132 -0.00240 2.05946

R11 3.32022 -0.00017 0.00065 -0.00743 -0.00677 3.31345

R12 3.38403 0.00051 0.00017 0.00958 0.00975 3.39379

R13 3.25537 -0.00039 -0.00084 -0.00453 -0.00537 3.24999

R14 3.47718 -0.00064 -0.00118 -0.00926 -0.01045 3.46673

R15 2.88244 -0.00047 -0.00089 0.00009 -0.00079 2.88165

R16 2.06503 -0.00025 -0.00073 0.00050 -0.00022 2.06481

R17 2.06183 -0.00052 -0.00109 -0.00200 -0.00308 2.05875

R18 2.89561 -0.00047 -0.00097 -0.00239 -0.00336 2.89225

R19 2.07349 -0.00044 -0.00074 -0.00253 -0.00327 2.07022

R20 2.07204 -0.00026 -0.00071 -0.00033 -0.00104 2.07101

R21 2.88754 -0.00045 -0.00097 0.00148 0.00051 2.88804

R22 2.07305 -0.00037 -0.00073 -0.00167 -0.00239 2.07065

R23 2.07284 -0.00034 -0.00072 -0.00164 -0.00236 2.07047

R24 2.06894 -0.00045 -0.00085 -0.00145 -0.00229 2.06665

R25 2.07026 -0.00034 -0.00070 -0.00194 -0.00263 2.06762

R26 2.07028 -0.00042 -0.00085 -0.00151 -0.00235 2.06792

A1 2.17633 0.00015 0.00085 0.00383 0.00469 2.18102

A2 1.97700 -0.00037 -0.00109 -0.00797 -0.00904 1.96797

A3 2.12888 0.00025 0.00062 0.00407 0.00470 2.13358

A4 2.02474 -0.00011 -0.00210 -0.00283 -0.00491 2.01983

A5 1.83565 -0.00049 0.00198 -0.00842 -0.00643 1.82922

A6 1.87423 -0.00004 -0.00183 0.00459 0.00275 1.87698

A7 1.94221 0.00079 0.00321 0.00678 0.00998 1.95219

A8 1.93773 0.00012 0.00153 0.00501 0.00655 1.94427

A9 1.83711 -0.00034 -0.00306 -0.00617 -0.00925 1.82786

A10 1.87791 -0.00114 -0.00242 -0.00542 -0.00784 1.87007

A11 1.90851 0.00058 0.00228 0.01108 0.01335 1.92186

A12 1.92816 -0.00009 -0.00014 -0.00593 -0.00608 1.92208

A13 1.95385 -0.00030 -0.00091 -0.00085 -0.00180 1.95205

A14 1.88496 -0.00024 -0.00090 -0.00294 -0.00382 1.88114

A15 1.89381 -0.00006 -0.00004 0.00151 0.00144 1.89525

A16 1.89297 0.00012 -0.00031 -0.00294 -0.00328 1.88969

A17 1.79405 0.00084 -0.00013 0.00325 0.00312 1.79717

A18 1.96973 0.00039 0.00089 -0.00649 -0.00557 1.96415

A19 2.14222 -0.00057 -0.00001 -0.00204 -0.00202 2.14020

A20 2.15160 0.00036 0.00136 0.00439 0.00577 2.15737

A21 1.79539 -0.00031 -0.00059 0.01002 0.00944 1.80483

A22 1.92767 -0.00042 -0.00093 -0.00825 -0.00924 1.91842

A23 1.87481 0.00042 0.00061 0.02058 0.02122 1.89603

A24 1.89552 -0.00016 -0.00028 -0.01587 -0.01624 1.87928

A25 1.93939 -0.00015 -0.00017 0.00228 0.00211 1.94150

A26 1.93739 0.00036 0.00088 -0.00098 -0.00023 1.93716

A27 1.88715 -0.00003 -0.00011 0.00271 0.00264 1.88980

A28 1.95403 -0.00016 -0.00015 0.00508 0.00491 1.95894

A29 1.91782 -0.00011 -0.00032 -0.01089 -0.01121 1.90661

A30 1.91510 0.00014 -0.00005 0.00865 0.00861 1.92370

A31 1.90534 0.00017 0.00066 0.00262 0.00329 1.90864

A32 1.90937 -0.00002 0.00005 -0.00437 -0.00436 1.90501

A33 1.85976 -0.00003 -0.00019 -0.00143 -0.00159 1.85816

A34 1.96702 -0.00025 -0.00036 -0.00477 -0.00514 1.96188

A35 1.90735 0.00003 -0.00075 0.00534 0.00460 1.91194

A36 1.90598 0.00014 0.00114 -0.00052 0.00062 1.90660

A37 1.91322 0.00006 -0.00046 0.00294 0.00248 1.91570

A38 1.91240 0.00006 0.00040 -0.00131 -0.00092 1.91149

A39 1.85446 -0.00003 0.00006 -0.00148 -0.00143 1.85303

A40 1.94590 -0.00010 -0.00026 0.00186 0.00160 1.94750

A41 1.94197 0.00003 0.00027 0.00230 0.00257 1.94453

A42 1.94278 0.00000 0.00028 -0.00519 -0.00491 1.93787

A43 1.87700 0.00003 -0.00037 0.00046 0.00008 1.87708

A44 1.87670 0.00007 0.00024 -0.00208 -0.00184 1.87486

A45 1.87610 -0.00002 -0.00018 0.00272 0.00254 1.87864

D1 2.70198 -0.00051 -0.03402 -0.00391 -0.03794 2.66404

D2 -1.42712 0.00006 -0.02973 -0.00345 -0.03317 -1.46029

D3 0.52339 -0.00056 -0.03306 -0.01224 -0.04530 0.47809

D4 -0.48624 0.00009 -0.02299 -0.00550 -0.02849 -0.51474

D5 1.66784 0.00066 -0.01870 -0.00504 -0.02372 1.64411

D6 -2.66483 0.00004 -0.02203 -0.01383 -0.03586 -2.70069

D7 -3.09561 -0.00031 -0.00803 0.00305 -0.00498 -3.10058

D8 0.00079 0.00027 0.00267 0.00151 0.00419 0.00498

D9 -3.13087 0.00000 0.00664 -0.06130 -0.05465 3.09767

D10 -1.05858 0.00000 0.00685 -0.06164 -0.05481 -1.11339

D11 1.05304 -0.00012 0.00574 -0.07009 -0.06435 0.98869

D12 1.05488 0.00011 0.00300 -0.05335 -0.05032 1.00456

D13 3.12717 0.00011 0.00322 -0.05370 -0.05048 3.07668

D14 -1.04439 -0.00001 0.00210 -0.06214 -0.06003 -1.10442

D15 -0.98522 -0.00004 0.00381 -0.05311 -0.04930 -1.03452

D16 1.08706 -0.00004 0.00402 -0.05345 -0.04946 1.03760

D17 -3.08450 -0.00016 0.00291 -0.06190 -0.05900 3.13969

D18 -3.11512 -0.00016 -0.02470 0.07729 0.05263 -3.06250

D19 -0.90924 -0.00014 -0.02393 0.07225 0.04832 -0.86092

D20 1.19131 0.00023 -0.02221 0.07819 0.05594 1.24725

D21 1.81758 0.00054 0.01633 -0.09390 -0.07755 1.74003

D22 -1.11850 -0.00045 0.00405 -0.07307 -0.06904 -1.18754

D23 2.56502 -0.00025 -0.00780 0.09057 0.08279 2.64781

D24 -0.78335 0.00061 0.00439 0.06873 0.07310 -0.71026

D25 -3.03553 0.00019 0.01237 -0.05533 -0.04287 -3.07841

D26 -0.91791 0.00002 0.01200 -0.04453 -0.03249 -0.95040

D27 1.11927 0.00012 0.01204 -0.03861 -0.02670 1.09257

D28 -3.10430 0.00008 -0.00398 -0.04350 -0.04748 3.13141

D29 -0.98399 0.00012 -0.00347 -0.04433 -0.04781 -1.03180

D30 1.05536 0.00011 -0.00391 -0.04736 -0.05131 1.00405

D31 1.10003 -0.00007 -0.00403 -0.06532 -0.06933 1.03070

D32 -3.06285 -0.00003 -0.00352 -0.06614 -0.06966 -3.13251

D33 -1.02350 -0.00005 -0.00397 -0.06917 -0.07316 -1.09666

D34 -1.00078 -0.00017 -0.00437 -0.06961 -0.07394 -1.07472

D35 1.11953 -0.00013 -0.00386 -0.07043 -0.07427 1.04526

D36 -3.12431 -0.00014 -0.00430 -0.07346 -0.07777 3.08111

D37 -3.11173 -0.00007 -0.00774 -0.03521 -0.04294 3.12851

D38 -0.98001 -0.00013 -0.00911 -0.03087 -0.03998 -1.01999

D39 1.04176 -0.00007 -0.00882 -0.02997 -0.03878 1.00298

D40 1.04398 0.00005 -0.00769 -0.02660 -0.03429 1.00969

D41 -3.10749 -0.00001 -0.00905 -0.02226 -0.03132 -3.13881

D42 -1.08572 0.00005 -0.00876 -0.02136 -0.03012 -1.11584

D43 -0.98491 0.00000 -0.00786 -0.02392 -0.03178 -1.01670

D44 1.14680 -0.00006 -0.00923 -0.01958 -0.02882 1.11798

D45 -3.11461 0.00000 -0.00894 -0.01867 -0.02762 3.14096

D46 -3.13259 -0.00006 -0.00674 0.02322 0.01648 -3.11611

D47 -1.03717 -0.00007 -0.00720 0.02663 0.01943 -1.01773

D48 1.05500 -0.00007 -0.00706 0.02813 0.02107 1.07608

D49 1.02219 0.00003 -0.00521 0.01754 0.01233 1.03453

D50 3.11762 0.00001 -0.00567 0.02095 0.01528 3.13290

D51 -1.07340 0.00001 -0.00552 0.02245 0.01692 -1.05648

D52 -1.00652 0.00000 -0.00524 0.01840 0.01316 -0.99336

D53 1.08890 -0.00002 -0.00570 0.02180 0.01611 1.10501

D54 -3.10211 -0.00002 -0.00556 0.02330 0.01775 -3.08436

Item Value Threshold Converged?

Maximum Force 0.002807 0.000450 NO

RMS Force 0.000452 0.000300 NO

Maximum Displacement 0.320902 0.001800 NO

RMS Displacement 0.107341 0.001200 NO

Predicted change in Energy=-1.029126D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:45:29 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.075221 -0.435209 -0.146664

2 6 0 -2.818293 0.071745 0.495549

3 8 0 -4.952682 0.262748 -0.597451

4 8 0 -4.118554 -1.782571 -0.217689

5 6 0 -2.188623 -0.846420 1.525455

6 16 0 -1.631859 0.425224 -0.963542

7 6 0 -0.143430 0.883965 -0.158217

8 16 0 1.041125 -0.463699 -0.081150

9 16 0 0.012944 2.341421 0.741316

10 6 0 2.661691 0.395535 -0.050834

11 6 0 3.792487 -0.627226 -0.075210

12 6 0 5.172458 0.034636 -0.065791

13 6 0 6.308776 -0.987325 -0.071686

14 1 0 -3.037288 1.050619 0.917442

15 1 0 -4.940716 -2.018694 -0.676731

16 1 0 -1.261502 -0.410717 1.899301

17 1 0 -2.863641 -0.976525 2.376539

18 1 0 -1.967942 -1.829873 1.110934

19 1 0 2.716875 1.067222 -0.910880

20 1 0 2.699786 0.997903 0.856130

21 1 0 3.700640 -1.287755 0.793934

22 1 0 3.706275 -1.266172 -0.961424

23 1 0 5.266629 0.698372 -0.932532

24 1 0 5.260020 0.674366 0.819377

25 1 0 7.287638 -0.500736 -0.038939

26 1 0 6.245692 -1.659816 0.789080

27 1 0 6.278873 -1.602657 -0.976096

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.499770 0.000000

3 O 1.208424 2.405567 0.000000

4 O 1.349929 2.374421 2.241276 0.000000

5 C 2.554277 1.516647 3.657459 2.763975 0.000000

6 S 2.716184 1.913510 3.344890 3.407977 2.849943

7 C 4.147208 2.870889 4.869060 4.787020 3.164143

8 S 5.116845 3.938831 6.059705 5.327321 3.627524

9 S 5.021083 3.636995 5.547128 5.915764 3.952734

10 C 6.788616 5.516665 7.635123 7.123461 5.249066

11 C 7.870376 6.672087 8.805838 7.996230 6.195471

12 C 9.259961 8.010530 10.141655 9.468274 7.582470

13 C 10.398936 9.205801 11.342820 10.458630 8.647342

14 H 2.101740 1.088185 2.566004 3.237996 2.165334

15 H 1.880818 3.201383 2.282850 0.970785 3.714547

16 H 3.479021 2.151019 4.506898 3.811348 1.090482

17 H 2.850878 2.153845 3.839857 2.992413 1.094038

18 H 2.822635 2.172084 4.025707 2.528361 1.089820

19 H 6.998135 5.797163 7.718000 7.438072 5.801867

20 H 6.997151 5.606869 7.823914 7.441362 5.267454

21 H 7.878806 6.665865 8.900562 7.899874 5.950910

22 H 7.868038 6.817828 8.800433 7.877040 6.411754

23 H 9.443133 8.233956 10.234079 9.733844 8.000554

24 H 9.450456 8.107228 10.318726 9.750368 7.635026

25 H 11.363558 10.136234 12.276819 11.479384 9.610741

26 H 10.435350 9.232567 11.446498 10.413753 8.505383

27 H 10.452663 9.366311 11.391705 10.426602 8.861611

6 7 8 9 10

6 S 0.000000

7 C 1.753400 0.000000

8 S 2.951888 1.795914 0.000000

9 S 3.046920 1.719823 3.098759 0.000000

10 C 4.389588 2.849350 1.834512 3.380804 0.000000

11 C 5.596455 4.216874 2.756224 4.874887 1.524905

12 C 6.874391 5.384103 4.161308 5.709051 2.536617

13 C 8.114455 6.718644 5.293621 7.167917 3.900509

14 H 2.429908 3.091801 4.463609 3.316792 5.817651

15 H 4.123534 5.631007 6.209279 6.749830 8.001052

16 H 3.005300 2.675755 3.037612 3.246444 4.454718

17 H 3.826007 4.157639 4.642244 4.685879 6.189022

18 H 3.082510 3.507778 3.513116 4.632518 5.266465

19 H 4.396182 2.963347 2.416672 3.415344 1.092651

20 H 4.733108 3.020887 2.401235 3.006217 1.089441

21 H 5.870141 4.516617 2.918537 5.174243 2.150933

22 H 5.599688 4.482015 2.919224 5.436428 2.163701

23 H 6.903963 5.468340 4.464319 5.753484 2.766731

24 H 7.123121 5.495169 4.461526 5.506085 2.754329

25 H 9.014971 7.559919 6.246765 7.849065 4.711987

26 H 8.335160 6.941835 5.410685 7.406709 4.216040

27 H 8.166525 6.935286 5.434350 7.600469 4.234724

11 12 13 14 15

11 C 0.000000

12 C 1.530513 0.000000

13 C 2.541927 1.528286 0.000000

14 H 7.102560 8.330601 9.616679 0.000000

15 H 8.863794 10.337587 11.312863 3.947797 0.000000

16 H 5.430320 6.742089 7.843875 2.500593 4.770549

17 H 7.101910 8.459688 9.493533 2.503683 3.837031

18 H 6.002987 7.473045 8.403127 3.078665 3.474015

19 H 2.174037 2.794691 4.222223 6.037668 8.259322

20 H 2.168509 2.809258 4.222178 5.737644 8.356242

21 H 1.095511 2.157335 2.764404 7.133227 8.796031

22 H 1.095929 2.154983 2.764489 7.373826 8.684342

23 H 2.159931 1.095743 2.160718 8.514783 10.565877

24 H 2.155940 1.095647 2.157568 8.306413 10.655792

25 H 3.497626 2.182046 1.093623 10.484535 12.338703

26 H 2.798474 2.180322 1.094139 9.671436 11.287742

27 H 2.818719 2.175670 1.094297 9.869966 11.231290

16 17 18 19 20

16 H 0.000000

17 H 1.764864 0.000000

18 H 1.770476 1.769812 0.000000

19 H 5.090078 6.791626 5.867572 0.000000

20 H 4.331768 6.096042 5.463417 1.768451 0.000000

21 H 5.158865 6.759534 5.703263 3.069218 2.495958

22 H 5.796064 7.374937 6.067056 2.534994 3.072875

23 H 7.201795 8.936248 7.931381 2.576386 3.142883

24 H 6.698797 8.434694 7.655041 3.100921 2.580857

25 H 8.766565 10.445543 9.420964 4.910259 4.908711

26 H 7.690956 9.271832 8.221697 4.772751 4.431864

27 H 8.157566 9.757960 8.509835 4.452004 4.788510

21 22 23 24 25

21 H 0.000000

22 H 1.755499 0.000000

23 H 3.062304 2.508978 0.000000

24 H 2.506438 3.057951 1.752086 0.000000

25 H 3.765584 3.776642 2.514129 2.495757 0.000000

26 H 2.572109 3.109318 3.079540 2.533945 1.764861

27 H 3.143160 2.594551 2.514214 3.073535 1.763547

26 27

26 H 0.000000

27 H 1.766413 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 5.06D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.072015 -0.521542 -0.068989

2 6 0 -2.811230 0.066253 0.491571

3 8 0 -4.953387 0.110390 -0.602031

4 8 0 -4.114301 -1.866454 0.039327

5 6 0 -2.173364 -0.707316 1.629523

6 16 0 -1.635378 0.223661 -1.009800

7 6 0 -0.141908 0.785315 -0.282817

8 16 0 1.044693 -0.540026 -0.036329

9 16 0 0.019054 2.349084 0.414685

10 6 0 2.664447 0.315998 -0.131472

11 6 0 3.796214 -0.700746 -0.028173

12 6 0 5.175461 -0.043173 -0.116198

13 6 0 6.312877 -1.056676 0.005274

14 1 0 -3.028404 1.092327 0.781666

15 1 0 -4.939366 -2.161456 -0.378603

16 1 0 -1.244163 -0.225750 1.935842

17 1 0 -2.842297 -0.723719 2.495074

18 1 0 -1.954448 -1.736952 1.347329

19 1 0 2.712881 0.867896 -1.073252

20 1 0 2.708162 1.033167 0.687454

21 1 0 3.711169 -1.240387 0.921406

22 1 0 3.704570 -1.451434 -0.821348

23 1 0 5.262842 0.499965 -1.063836

24 1 0 5.268446 0.708153 0.675827

25 1 0 7.291386 -0.569829 -0.033596

26 1 0 6.256550 -1.609278 0.947929

27 1 0 6.277387 -1.786356 -0.809462

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2600931 0.1969406 0.1824783

Leave Link 202 at Sat Aug 17 17:45:29 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1104.4232431129 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0551353298 Hartrees.

Nuclear repulsion after empirical dispersion term = 1104.3681077831 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

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Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2322

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.35D-09

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 99

GePol: Fraction of low-weight points (<1% of avg) = 4.26%

GePol: Cavity surface area = 307.789 Ang\*\*2

GePol: Cavity volume = 320.053 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0056764752 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1104.3624313079 Hartrees.

Leave Link 301 at Sat Aug 17 17:45:30 2019, MaxMem= 1342177280 cpu: 1.0

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 296 296 296 296 296 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:45:30 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:45:30 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999818 -0.018927 -0.002151 -0.000982 Ang= -2.19 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.63022607200

Leave Link 401 at Sat Aug 17 17:45:30 2019, MaxMem= 1342177280 cpu: 7.6

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16175052.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.55D-15 for 2295.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.10D-15 for 969 9.

Iteration 1 A^-1\*A deviation from unit magnitude is 4.66D-15 for 2295.

Iteration 1 A^-1\*A deviation from orthogonality is 1.02D-07 for 741 731.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.66D-15 for 18.

Iteration 2 A\*A^-1 deviation from orthogonality is 2.89D-15 for 1456 1122.

Iteration 2 A^-1\*A deviation from unit magnitude is 8.88D-16 for 151.

Iteration 2 A^-1\*A deviation from orthogonality is 4.19D-16 for 206 193.

E= -1658.65319766414

DIIS: error= 5.52D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.65319766414 IErMin= 1 ErrMin= 5.52D-03

ErrMax= 5.52D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.23D-02 BMatP= 5.23D-02

IDIUse=3 WtCom= 9.45D-01 WtEn= 5.52D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.429 Goal= None Shift= 0.000

Gap= 0.484 Goal= None Shift= 0.000

GapD= 0.429 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=5.53D-04 MaxDP=1.42D-02 OVMax= 3.04D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 5.53D-04 CP: 9.99D-01

E= -1658.67634082109 Delta-E= -0.023143156946 Rises=F Damp=F

DIIS: error= 8.16D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67634082109 IErMin= 2 ErrMin= 8.16D-04

ErrMax= 8.16D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.11D-03 BMatP= 5.23D-02

IDIUse=3 WtCom= 9.92D-01 WtEn= 8.16D-03

Coeff-Com: -0.584D-01 0.106D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.579D-01 0.106D+01

Gap= 0.124 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=9.16D-05 MaxDP=3.36D-03 DE=-2.31D-02 OVMax= 5.14D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 8.74D-05 CP: 9.99D-01 1.05D+00

E= -1658.67653345321 Delta-E= -0.000192632114 Rises=F Damp=F

DIIS: error= 1.10D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67653345321 IErMin= 2 ErrMin= 8.16D-04

ErrMax= 1.10D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.03D-04 BMatP= 1.11D-03

IDIUse=3 WtCom= 9.89D-01 WtEn= 1.10D-02

Coeff-Com: -0.380D-01 0.510D+00 0.528D+00

Coeff-En: 0.000D+00 0.793D-01 0.921D+00

Coeff: -0.375D-01 0.505D+00 0.533D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.51D-05 MaxDP=2.66D-03 DE=-1.93D-04 OVMax= 5.47D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 4.06D-05 CP: 9.99D-01 1.08D+00 6.24D-01

E= -1658.67666423634 Delta-E= -0.000130783132 Rises=F Damp=F

DIIS: error= 3.94D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67666423634 IErMin= 4 ErrMin= 3.94D-04

ErrMax= 3.94D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.80D-04 BMatP= 8.03D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.94D-03

Coeff-Com: -0.126D-01 0.160D+00 0.334D+00 0.518D+00

Coeff-En: 0.000D+00 0.000D+00 0.186D+00 0.814D+00

Coeff: -0.126D-01 0.160D+00 0.334D+00 0.519D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=2.13D-05 MaxDP=1.06D-03 DE=-1.31D-04 OVMax= 1.72D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.45D-05 CP: 9.99D-01 1.09D+00 7.00D-01 6.67D-01

E= -1658.67669917605 Delta-E= -0.000034939715 Rises=F Damp=F

DIIS: error= 1.24D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67669917605 IErMin= 5 ErrMin= 1.24D-04

ErrMax= 1.24D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.27D-05 BMatP= 1.80D-04

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.24D-03

Coeff-Com: -0.424D-02 0.504D-01 0.155D+00 0.299D+00 0.500D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.423D-02 0.504D-01 0.155D+00 0.298D+00 0.500D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=6.74D-06 MaxDP=2.92D-04 DE=-3.49D-05 OVMax= 6.63D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 4.36D-06 CP: 9.99D-01 1.09D+00 7.11D-01 7.68D-01 8.01D-01

E= -1658.67670182103 Delta-E= -0.000002644982 Rises=F Damp=F

DIIS: error= 4.53D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67670182103 IErMin= 6 ErrMin= 4.53D-05

ErrMax= 4.53D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.67D-06 BMatP= 1.27D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.316D-03-0.868D-02 0.190D-01 0.629D-01 0.285D+00 0.642D+00

Coeff: 0.316D-03-0.868D-02 0.190D-01 0.629D-01 0.285D+00 0.642D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=2.67D-06 MaxDP=8.93D-05 DE=-2.64D-06 OVMax= 3.58D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.76D-06 CP: 9.99D-01 1.09D+00 7.28D-01 7.86D-01 8.67D-01

CP: 9.00D-01

E= -1658.67670221306 Delta-E= -0.000000392029 Rises=F Damp=F

DIIS: error= 1.26D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67670221306 IErMin= 7 ErrMin= 1.26D-05

ErrMax= 1.26D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.57D-07 BMatP= 1.67D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.651D-03-0.105D-01-0.903D-02-0.456D-02 0.765D-01 0.300D+00

Coeff-Com: 0.647D+00

Coeff: 0.651D-03-0.105D-01-0.903D-02-0.456D-02 0.765D-01 0.300D+00

Coeff: 0.647D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=1.21D-06 MaxDP=4.39D-05 DE=-3.92D-07 OVMax= 1.82D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 7.30D-07 CP: 9.99D-01 1.09D+00 7.30D-01 8.00D-01 9.08D-01

CP: 9.88D-01 1.03D+00

E= -1658.67670226267 Delta-E= -0.000000049612 Rises=F Damp=F

DIIS: error= 5.67D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67670226267 IErMin= 8 ErrMin= 5.67D-06

ErrMax= 5.67D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.51D-08 BMatP= 1.57D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.201D-03-0.260D-02-0.551D-02-0.972D-02-0.971D-02 0.255D-01

Coeff-Com: 0.285D+00 0.716D+00

Coeff: 0.201D-03-0.260D-02-0.551D-02-0.972D-02-0.971D-02 0.255D-01

Coeff: 0.285D+00 0.716D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=6.82D-07 MaxDP=2.51D-05 DE=-4.96D-08 OVMax= 1.07D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 3.34D-07 CP: 9.99D-01 1.09D+00 7.30D-01 8.08D-01 9.22D-01

CP: 1.06D+00 1.18D+00 1.06D+00

E= -1658.67670227217 Delta-E= -0.000000009496 Rises=F Damp=F

DIIS: error= 3.59D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67670227217 IErMin= 9 ErrMin= 3.59D-06

ErrMax= 3.59D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.01D-08 BMatP= 2.51D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.263D-04 0.909D-03-0.143D-02-0.552D-02-0.257D-01-0.570D-01

Coeff-Com: 0.274D-01 0.449D+00 0.612D+00

Coeff: -0.263D-04 0.909D-03-0.143D-02-0.552D-02-0.257D-01-0.570D-01

Coeff: 0.274D-01 0.449D+00 0.612D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=3.07D-07 MaxDP=1.41D-05 DE=-9.50D-09 OVMax= 5.43D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.50D-07 CP: 9.99D-01 1.09D+00 7.31D-01 8.10D-01 9.30D-01

CP: 1.08D+00 1.27D+00 1.18D+00 8.05D-01

E= -1658.67670227547 Delta-E= -0.000000003299 Rises=F Damp=F

DIIS: error= 1.53D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67670227547 IErMin=10 ErrMin= 1.53D-06

ErrMax= 1.53D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.08D-09 BMatP= 1.01D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.612D-04 0.116D-02 0.306D-03-0.136D-02-0.142D-01-0.410D-01

Coeff-Com: -0.505D-01 0.105D+00 0.377D+00 0.624D+00

Coeff: -0.612D-04 0.116D-02 0.306D-03-0.136D-02-0.142D-01-0.410D-01

Coeff: -0.505D-01 0.105D+00 0.377D+00 0.624D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=1.59D-07 MaxDP=5.13D-06 DE=-3.30D-09 OVMax= 2.24D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 6.78D-08 CP: 9.99D-01 1.09D+00 7.32D-01 8.11D-01 9.30D-01

CP: 1.09D+00 1.31D+00 1.28D+00 9.70D-01 8.13D-01

E= -1658.67670227622 Delta-E= -0.000000000750 Rises=F Damp=F

DIIS: error= 3.61D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67670227622 IErMin=11 ErrMin= 3.61D-07

ErrMax= 3.61D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.95D-10 BMatP= 2.08D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.209D-04 0.320D-03 0.341D-03 0.337D-03-0.165D-02-0.687D-02

Coeff-Com: -0.241D-01-0.264D-01 0.628D-01 0.264D+00 0.732D+00

Coeff: -0.209D-04 0.320D-03 0.341D-03 0.337D-03-0.165D-02-0.687D-02

Coeff: -0.241D-01-0.264D-01 0.628D-01 0.264D+00 0.732D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=4.93D-08 MaxDP=2.82D-06 DE=-7.50D-10 OVMax= 5.58D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 3.15D-08 CP: 9.99D-01 1.09D+00 7.32D-01 8.12D-01 9.30D-01

CP: 1.09D+00 1.32D+00 1.29D+00 1.03D+00 9.38D-01

CP: 9.48D-01

E= -1658.67670227627 Delta-E= -0.000000000049 Rises=F Damp=F

DIIS: error= 1.82D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.67670227627 IErMin=12 ErrMin= 1.82D-07

ErrMax= 1.82D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.88D-11 BMatP= 1.95D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.247D-05-0.913D-04 0.114D-03 0.486D-03 0.234D-02 0.571D-02

Coeff-Com: -0.211D-02-0.399D-01-0.507D-01-0.329D-02 0.397D+00 0.690D+00

Coeff: 0.247D-05-0.913D-04 0.114D-03 0.486D-03 0.234D-02 0.571D-02

Coeff: -0.211D-02-0.399D-01-0.507D-01-0.329D-02 0.397D+00 0.690D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=2.30D-08 MaxDP=1.05D-06 DE=-4.91D-11 OVMax= 1.82D-06

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.08D-08 CP: 9.99D-01 1.09D+00 7.32D-01 8.12D-01 9.30D-01

CP: 1.09D+00 1.32D+00 1.30D+00 1.05D+00 9.94D-01

CP: 1.16D+00 8.32D-01

E= -1658.67670227631 Delta-E= -0.000000000040 Rises=F Damp=F

DIIS: error= 5.62D-08 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1658.67670227631 IErMin=13 ErrMin= 5.62D-08

ErrMax= 5.62D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.23D-12 BMatP= 5.88D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.317D-05-0.628D-04-0.766D-05 0.101D-03 0.822D-03 0.238D-02

Coeff-Com: 0.250D-02-0.714D-02-0.195D-01-0.350D-01 0.821D-02 0.168D+00

Coeff-Com: 0.880D+00

Coeff: 0.317D-05-0.628D-04-0.766D-05 0.101D-03 0.822D-03 0.238D-02

Coeff: 0.250D-02-0.714D-02-0.195D-01-0.350D-01 0.821D-02 0.168D+00

Coeff: 0.880D+00

Gap= 0.123 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=8.44D-09 MaxDP=3.01D-07 DE=-3.96D-11 OVMax= 8.80D-07

Error on total polarization charges = 0.04160

SCF Done: E(UB3LYP) = -1658.67670228 A.U. after 13 cycles

NFock= 13 Conv=0.84D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7551 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655272602998D+03 PE=-6.151518947879D+03 EE= 1.733207211297D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.56

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7551, after 0.7500

Leave Link 502 at Sat Aug 17 17:45:59 2019, MaxMem= 1342177280 cpu: 335.4

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 333

Leave Link 701 at Sat Aug 17 17:46:00 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:46:00 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:46:04 2019, MaxMem= 1342177280 cpu: 38.5

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.51098644D+00-3.11439957D+00 5.88299904D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.004405681 -0.001376090 0.002579853

2 6 0.000338715 0.000753658 -0.000229662

3 8 -0.003379314 0.002290536 -0.002023244

4 8 -0.000969373 -0.000918513 -0.000207015

5 6 -0.000163997 0.000086255 -0.000209531

6 16 0.000313708 -0.000905959 0.000041824

7 6 0.000202297 -0.001097279 0.000449636

8 16 -0.000820539 0.000041548 -0.001534050

9 16 0.000628841 0.000791169 0.000209097

10 6 0.000270742 -0.000145387 0.000611209

11 6 -0.000096864 0.000160483 -0.000312962

12 6 0.000523940 -0.000359868 0.001598406

13 6 -0.000063242 0.000869497 -0.001166068

14 1 -0.000249045 0.000289843 0.000565786

15 1 -0.000952368 -0.000814602 -0.000590707

16 1 -0.000194845 0.000375564 -0.000173200

17 1 -0.000435643 -0.000207849 0.000438620

18 1 0.000477463 0.000086155 -0.000183401

19 1 -0.000771555 -0.000244985 -0.000186470

20 1 0.000995616 0.000923943 0.000006225

21 1 0.000492901 -0.000564944 0.000343733

22 1 -0.000461220 0.000228011 -0.000338319

23 1 -0.000071450 -0.000112919 -0.000453858

24 1 0.000026766 0.000320012 0.000513363

25 1 0.000187759 0.000356646 -0.000043157

26 1 -0.000246895 -0.000150757 0.000385819

27 1 0.000011922 -0.000674167 -0.000091926

-------------------------------------------------------------------

Cartesian Forces: Max 0.004405681 RMS 0.000941723

Leave Link 716 at Sat Aug 17 17:46:04 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.004537237 RMS 0.000832589

Search for a local minimum.

Step number 35 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .83259D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 33 34 35

DE= 2.44D-04 DEPred=-1.03D-04 R=-2.37D+00

Trust test=-2.37D+00 RLast= 3.53D-01 DXMaxT set to 5.00D-02

ITU= -1 -1 0 -1 0 0 -1 -1 0 0 -1 0 0 -1 1 -1 1 -1 1 1

ITU= -1 1 -1 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Eigenvalues --- 0.00019 0.00159 0.00250 0.00289 0.00305

Eigenvalues --- 0.00419 0.00504 0.00844 0.01480 0.02309

Eigenvalues --- 0.02970 0.03531 0.03544 0.04438 0.04767

Eigenvalues --- 0.04822 0.04878 0.05056 0.05183 0.05464

Eigenvalues --- 0.05465 0.05607 0.05688 0.05836 0.08137

Eigenvalues --- 0.08293 0.08337 0.11069 0.11930 0.12157

Eigenvalues --- 0.13309 0.14506 0.15627 0.15979 0.16022

Eigenvalues --- 0.16046 0.16177 0.16314 0.16856 0.17063

Eigenvalues --- 0.19409 0.20284 0.21888 0.22237 0.23168

Eigenvalues --- 0.24407 0.25129 0.25404 0.26398 0.26443

Eigenvalues --- 0.27578 0.28314 0.29083 0.29468 0.29676

Eigenvalues --- 0.30716 0.32396 0.32519 0.33643 0.33876

Eigenvalues --- 0.33892 0.33908 0.33951 0.34041 0.34051

Eigenvalues --- 0.34118 0.34229 0.34351 0.34610 0.34708

Eigenvalues --- 0.35042 0.36451 0.52642 0.56768 0.99822

En-DIIS/RFO-DIIS IScMMF= 0 using points: 35 34 33

RFO step: Lambda=-1.88628379D-04.

NNeg= 0 NP= 3 Switch= 2.50D-03 Rises=T DC= -3.43D-05 SmlDif= 1.00D-05

RMS Error= 0.2753744368D-02 NUsed= 3 EDIIS=F

DidBck=T Rises=T RFO-DIIS coefs: 0.19103 0.68076 0.12821

Iteration 1 RMS(Cart)= 0.23224208 RMS(Int)= 0.05372794

Iteration 2 RMS(Cart)= 0.07268843 RMS(Int)= 0.00833116

Iteration 3 RMS(Cart)= 0.01057034 RMS(Int)= 0.00051591

Iteration 4 RMS(Cart)= 0.00018441 RMS(Int)= 0.00049131

Iteration 5 RMS(Cart)= 0.00000006 RMS(Int)= 0.00049131

ITry= 1 IFail=0 DXMaxC= 1.28D+00 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83415 0.00114 0.00510 -0.00733 -0.00223 2.83192

R2 2.28359 0.00454 0.00625 -0.01759 -0.01134 2.27225

R3 2.55100 0.00182 0.00388 -0.00770 -0.00382 2.54718

R4 2.86605 -0.00044 0.00063 -0.01311 -0.01248 2.85357

R5 3.61601 0.00052 -0.01221 0.03303 0.02083 3.63684

R6 2.05637 0.00053 0.00212 -0.00322 -0.00110 2.05527

R7 1.83452 0.00129 0.00300 -0.00664 -0.00364 1.83088

R8 2.06071 -0.00008 0.00096 -0.00474 -0.00379 2.05693

R9 2.06743 0.00063 0.00167 -0.00641 -0.00474 2.06269

R10 2.05946 0.00009 0.00174 -0.00472 -0.00298 2.05648

R11 3.31345 0.00080 0.00560 -0.02862 -0.02302 3.29043

R12 3.39379 -0.00051 -0.00786 0.00021 -0.00764 3.38614

R13 3.24999 0.00084 0.00419 -0.00619 -0.00200 3.24800

R14 3.46673 0.00100 0.00823 -0.00267 0.00556 3.47229

R15 2.88165 0.00019 0.00047 -0.00859 -0.00811 2.87354

R16 2.06481 -0.00005 0.00004 -0.00500 -0.00496 2.05985

R17 2.05875 0.00056 0.00229 -0.00570 -0.00341 2.05534

R18 2.89225 0.00044 0.00254 -0.00420 -0.00166 2.89059

R19 2.07022 0.00057 0.00251 -0.00473 -0.00222 2.06800

R20 2.07101 0.00018 0.00071 -0.00407 -0.00336 2.06765

R21 2.88804 -0.00034 -0.00059 -0.00682 -0.00741 2.88063

R22 2.07065 0.00028 0.00180 -0.00450 -0.00270 2.06796

R23 2.07047 0.00061 0.00178 -0.00377 -0.00199 2.06848

R24 2.06665 0.00032 0.00170 -0.00454 -0.00285 2.06380

R25 2.06762 0.00041 0.00200 -0.00467 -0.00267 2.06496

R26 2.06792 0.00045 0.00174 -0.00410 -0.00235 2.06557

A1 2.18102 -0.00079 -0.00363 -0.00535 -0.00900 2.17202

A2 1.96797 0.00248 0.00711 0.00276 0.00985 1.97781

A3 2.13358 -0.00169 -0.00369 0.00229 -0.00142 2.13216

A4 2.01983 0.00078 0.00357 0.03077 0.03395 2.05378

A5 1.82922 -0.00035 0.00557 -0.05253 -0.04669 1.78253

A6 1.87698 -0.00040 -0.00257 0.00776 0.00496 1.88194

A7 1.95219 -0.00009 -0.00747 -0.00390 -0.01100 1.94119

A8 1.94427 -0.00030 -0.00501 0.00350 -0.00186 1.94242

A9 1.82786 0.00031 0.00691 0.01038 0.01734 1.84520

A10 1.87007 0.00093 0.00589 -0.01560 -0.00971 1.86037

A11 1.92186 -0.00069 -0.01037 0.00563 -0.00474 1.91712

A12 1.92208 0.00020 0.00489 0.00288 0.00777 1.92985

A13 1.95205 0.00007 0.00128 0.00073 0.00202 1.95408

A14 1.88114 0.00021 0.00292 0.00033 0.00324 1.88438

A15 1.89525 0.00015 -0.00117 -0.00301 -0.00416 1.89109

A16 1.88969 0.00008 0.00260 -0.00685 -0.00424 1.88544

A17 1.79717 0.00361 -0.00255 0.02448 0.02194 1.81910

A18 1.96415 0.00091 0.00468 0.01733 0.01891 1.98306

A19 2.14020 0.00038 0.00163 -0.00005 -0.00153 2.13867

A20 2.15737 -0.00076 -0.00441 0.00905 0.00154 2.15891

A21 1.80483 -0.00224 -0.00774 -0.00686 -0.01461 1.79022

A22 1.91842 0.00120 0.00730 0.01057 0.01789 1.93632

A23 1.89603 -0.00123 -0.01705 0.00156 -0.01550 1.88053

A24 1.87928 0.00057 0.01308 -0.01120 0.00183 1.88111

A25 1.94150 -0.00003 -0.00174 0.00002 -0.00167 1.93983

A26 1.93716 -0.00049 0.00035 0.00088 0.00126 1.93841

A27 1.88980 -0.00004 -0.00216 -0.00236 -0.00457 1.88523

A28 1.95894 -0.00075 -0.00400 -0.00811 -0.01210 1.94684

A29 1.90661 0.00090 0.00901 0.00175 0.01074 1.91735

A30 1.92370 -0.00043 -0.00697 0.00560 -0.00137 1.92233

A31 1.90864 -0.00025 -0.00254 0.00192 -0.00060 1.90804

A32 1.90501 0.00064 0.00354 0.00257 0.00612 1.91113

A33 1.85816 -0.00008 0.00125 -0.00350 -0.00227 1.85590

A34 1.96188 0.00065 0.00409 0.00143 0.00551 1.96739

A35 1.91194 -0.00044 -0.00386 0.00060 -0.00325 1.90869

A36 1.90660 -0.00005 -0.00028 -0.00017 -0.00047 1.90613

A37 1.91570 -0.00033 -0.00210 -0.00021 -0.00230 1.91340

A38 1.91149 -0.00007 0.00082 0.00243 0.00324 1.91473

A39 1.85303 0.00021 0.00116 -0.00441 -0.00325 1.84978

A40 1.94750 -0.00030 -0.00134 0.00120 -0.00014 1.94736

A41 1.94453 -0.00044 -0.00203 0.00190 -0.00013 1.94441

A42 1.93787 0.00059 0.00403 0.00333 0.00735 1.94522

A43 1.87708 0.00030 -0.00014 -0.00016 -0.00029 1.87679

A44 1.87486 0.00003 0.00153 -0.00397 -0.00244 1.87242

A45 1.87864 -0.00016 -0.00209 -0.00274 -0.00483 1.87381

D1 2.66404 0.00007 0.02430 0.41022 0.43477 3.09881

D2 -1.46029 0.00019 0.02125 0.38520 0.40626 -1.05403

D3 0.47809 0.00022 0.03044 0.37688 0.40723 0.88532

D4 -0.51474 0.00006 0.01873 0.40133 0.42033 -0.09441

D5 1.64411 0.00018 0.01568 0.37631 0.39182 2.03593

D6 -2.70069 0.00021 0.02487 0.36799 0.39279 -2.30790

D7 -3.10058 0.00004 0.00252 0.02864 0.03119 -3.06939

D8 0.00498 0.00005 -0.00289 0.01984 0.01693 0.02191

D9 3.09767 0.00018 0.04545 -0.05605 -0.01071 3.08696

D10 -1.11339 0.00014 0.04562 -0.05038 -0.00485 -1.11824

D11 0.98869 0.00042 0.05313 -0.05659 -0.00355 0.98514

D12 1.00456 0.00014 0.04127 -0.00567 0.03564 1.04020

D13 3.07668 0.00010 0.04144 0.00000 0.04150 3.11818

D14 -1.10442 0.00038 0.04895 -0.00621 0.04279 -1.06163

D15 -1.03452 0.00001 0.04060 -0.01846 0.02218 -1.01234

D16 1.03760 -0.00004 0.04076 -0.01278 0.02804 1.06565

D17 3.13969 0.00024 0.04827 -0.01899 0.02934 -3.11416

D18 -3.06250 -0.00055 -0.04721 0.22791 0.18022 -2.88227

D19 -0.86092 0.00013 -0.04359 0.22751 0.18430 -0.67662

D20 1.24725 -0.00009 -0.04942 0.23608 0.18677 1.43401

D21 1.74003 0.00263 0.06581 -0.04624 0.01960 1.75962

D22 -1.18754 0.00012 0.05661 -0.17692 -0.12033 -1.30787

D23 2.64781 -0.00137 -0.06844 0.01688 -0.05175 2.59606

D24 -0.71026 0.00134 -0.05831 0.14777 0.08965 -0.62061

D25 -3.07841 0.00041 0.03701 0.17571 0.21272 -2.86568

D26 -0.95040 0.00034 0.02854 0.18332 0.21177 -0.73864

D27 1.09257 -0.00005 0.02386 0.17530 0.19925 1.29182

D28 3.13141 -0.00052 0.03766 -0.00350 0.03417 -3.11761

D29 -1.03180 -0.00070 0.03802 -0.00520 0.03280 -0.99901

D30 1.00405 -0.00051 0.04077 -0.00519 0.03558 1.03963

D31 1.03070 0.00024 0.05533 -0.01247 0.04286 1.07356

D32 -3.13251 0.00006 0.05569 -0.01418 0.04149 -3.09102

D33 -1.09666 0.00025 0.05844 -0.01417 0.04427 -1.05238

D34 -1.07472 0.00065 0.05900 -0.01009 0.04893 -1.02580

D35 1.04526 0.00047 0.05936 -0.01180 0.04755 1.09281

D36 3.08111 0.00065 0.06211 -0.01178 0.05034 3.13145

D37 3.12851 0.00063 0.03329 -0.03582 -0.00252 3.12599

D38 -1.01999 0.00033 0.03063 -0.03468 -0.00405 -1.02404

D39 1.00298 0.00032 0.02971 -0.03974 -0.01001 0.99297

D40 1.00969 0.00015 0.02629 -0.03400 -0.00771 1.00198

D41 -3.13881 -0.00014 0.02364 -0.03287 -0.00923 3.13514

D42 -1.11584 -0.00016 0.02272 -0.03792 -0.01520 -1.13104

D43 -1.01670 0.00003 0.02424 -0.03233 -0.00810 -1.02479

D44 1.11798 -0.00027 0.02158 -0.03119 -0.00962 1.10837

D45 3.14096 -0.00029 0.02066 -0.03625 -0.01559 3.12537

D46 -3.11611 -0.00019 -0.01460 0.00131 -0.01329 -3.12940

D47 -1.01773 -0.00032 -0.01707 0.00323 -0.01385 -1.03158

D48 1.07608 -0.00043 -0.01837 0.00328 -0.01509 1.06098

D49 1.03453 0.00016 -0.01095 -0.00029 -0.01124 1.02328

D50 3.13290 0.00003 -0.01343 0.00163 -0.01180 3.12110

D51 -1.05648 -0.00007 -0.01473 0.00168 -0.01305 -1.06952

D52 -0.99336 0.00014 -0.01163 0.00375 -0.00787 -1.00123

D53 1.10501 0.00000 -0.01410 0.00568 -0.00842 1.09659

D54 -3.08436 -0.00010 -0.01540 0.00573 -0.00967 -3.09403

Item Value Threshold Converged?

Maximum Force 0.004537 0.000450 NO

RMS Force 0.000833 0.000300 NO

Maximum Displacement 1.277092 0.001800 NO

RMS Displacement 0.266459 0.001200 NO

Predicted change in Energy=-4.649986D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:46:04 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -3.970230 -0.559059 -0.342127

2 6 0 -2.884118 0.119667 0.435985

3 8 0 -4.549683 -0.066063 -1.273259

4 8 0 -4.205455 -1.823446 0.061426

5 6 0 -2.298367 -0.620501 1.614661

6 16 0 -1.554049 0.436874 -0.918309

7 6 0 -0.112324 0.820730 -0.020572

8 16 0 1.036622 -0.547895 0.112023

9 16 0 0.117050 2.336937 0.755739

10 6 0 2.665175 0.301122 0.168847

11 6 0 3.797414 -0.676010 -0.105945

12 6 0 5.162493 0.009816 -0.028621

13 6 0 6.319196 -0.951019 -0.278662

14 1 0 -3.247778 1.102261 0.727778

15 1 0 -4.869560 -2.187650 -0.542736

16 1 0 -1.487988 -0.038990 2.050456

17 1 0 -3.055364 -0.773836 2.385945

18 1 0 -1.906108 -1.594669 1.329356

19 1 0 2.648495 1.101666 -0.570755

20 1 0 2.769573 0.753835 1.152262

21 1 0 3.763299 -1.497186 0.616604

22 1 0 3.672086 -1.129778 -1.093647

23 1 0 5.199637 0.826942 -0.755568

24 1 0 5.276112 0.476148 0.955127

25 1 0 7.284321 -0.444939 -0.207004

26 1 0 6.321871 -1.769062 0.445805

27 1 0 6.259841 -1.397533 -1.274586

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.498588 0.000000

3 O 1.202422 2.393766 0.000000

4 O 1.347909 2.379478 2.233444 0.000000

5 C 2.574475 1.510043 3.703500 2.737992 0.000000

6 S 2.676154 1.924531 3.058229 3.619238 2.843939

7 C 4.109824 2.895302 4.695294 4.873614 3.087056

8 S 5.027420 3.990338 5.775637 5.395273 3.658599

9 S 5.128154 3.745069 5.627579 6.039446 3.913876

10 C 6.710410 5.558682 7.366728 7.192419 5.251335

11 C 7.772114 6.750530 8.450366 8.086441 6.334201

12 C 9.155793 8.060762 9.791897 9.546068 7.665644

13 C 10.297084 9.292905 10.950110 10.566223 8.829286

14 H 2.103953 1.087604 2.657835 3.149751 2.157742

15 H 1.871188 3.197434 2.266520 0.968861 3.704234

16 H 3.486610 2.140296 4.519047 3.811187 1.088478

17 H 2.885392 2.151747 4.015433 2.797817 1.091529

18 H 2.850779 2.166463 4.012322 2.635712 1.088241

19 H 6.827723 5.708560 7.326041 7.478808 5.675680

20 H 7.027221 5.734061 7.754154 7.515539 5.271302

21 H 7.848994 6.843609 8.644383 7.994730 6.205520

22 H 7.700357 6.847241 8.292240 7.991935 6.575759

23 H 9.283232 8.201655 9.803811 9.805498 7.995820

24 H 9.394113 8.184494 10.089893 9.797293 7.681819

25 H 11.255940 10.204380 11.887981 11.575288 9.755879

26 H 10.392896 9.397746 11.137598 10.534482 8.774618

27 H 10.306642 9.425494 10.891218 10.558823 9.066115

6 7 8 9 10

6 S 0.000000

7 C 1.741220 0.000000

8 S 2.956845 1.791869 0.000000

9 S 3.034015 1.718765 3.095519 0.000000

10 C 4.359150 2.832027 1.837456 3.313898 0.000000

11 C 5.525993 4.187311 2.772344 4.833779 1.520612

12 C 6.788657 5.336792 4.165769 5.611346 2.521993

13 C 8.020185 6.676088 5.312318 7.095579 3.888443

14 H 2.453785 3.235793 4.632306 3.584310 5.993099

15 H 4.245209 5.652813 6.164454 6.857419 7.966967

16 H 3.007387 2.630727 3.223378 3.146024 4.572187

17 H 3.825946 4.122553 4.686803 4.732725 6.228613

18 H 3.050100 3.297593 3.352208 4.458669 5.083054

19 H 4.268971 2.829090 2.405280 3.113469 1.090027

20 H 4.804314 3.112129 2.404104 3.114373 1.087637

21 H 5.862656 4.560612 2.930959 5.292918 2.154130

22 H 5.458720 4.390642 2.955993 5.298738 2.157600

23 H 6.766898 5.362573 4.469181 5.513332 2.748550

24 H 7.082542 5.486891 4.442157 5.488006 2.732373

25 H 8.910686 7.506466 6.256685 7.748256 4.694079

26 H 8.291989 6.951503 5.434751 7.446817 4.211151

27 H 8.034230 6.862779 5.470519 7.470098 4.229722

11 12 13 14 15

11 C 0.000000

12 C 1.529633 0.000000

13 C 2.542606 1.524364 0.000000

14 H 7.313827 8.514589 9.836456 0.000000

15 H 8.808648 10.282765 11.259984 3.881739 0.000000

16 H 5.743809 6.968059 8.198092 2.479675 4.772464

17 H 7.292438 8.601012 9.747507 2.511231 3.723889

18 H 5.952662 7.374524 8.405690 3.071710 3.555052

19 H 2.167071 2.793964 4.215789 6.037567 8.206188

20 H 2.164254 2.770219 4.189736 6.042359 8.359528

21 H 1.094336 2.155253 2.762681 7.478280 8.737680

22 H 1.094151 2.157375 2.775490 7.495606 8.624518

23 H 2.155714 1.094315 2.154528 8.581080 10.512934

24 H 2.154040 1.094593 2.155705 8.549877 10.595946

25 H 3.496016 2.177332 1.092116 10.686101 12.282775

26 H 2.805722 2.175694 1.092728 9.995108 11.242800

27 H 2.819550 2.176518 1.093052 10.032609 11.181388

16 17 18 19 20

16 H 0.000000

17 H 1.763297 0.000000

18 H 1.764921 1.763785 0.000000

19 H 5.028154 6.692801 5.623616 0.000000

20 H 4.422912 6.147003 5.235344 1.761941 0.000000

21 H 5.635449 7.081522 5.714866 3.067025 2.518236

22 H 6.140160 7.582403 6.099452 2.510080 3.067024

23 H 7.303968 8.976449 7.791196 2.572539 3.090367

24 H 6.871547 8.545360 7.484158 3.102251 2.529567

25 H 9.067212 10.664925 9.388624 4.900529 4.864936

26 H 8.158551 9.627417 8.277120 4.771600 4.413945

27 H 8.539930 10.028037 8.573337 4.447831 4.764446

21 22 23 24 25

21 H 0.000000

22 H 1.751647 0.000000

23 H 3.057367 2.505287 0.000000

24 H 2.509431 3.057674 1.747965 0.000000

25 H 3.766052 3.781981 2.502900 2.496368 0.000000

26 H 2.578640 3.130488 3.072774 2.528633 1.762320

27 H 3.133569 2.607855 2.518273 3.074089 1.759752

26 27

26 H 0.000000

27 H 1.761144 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 8.50D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.015273 -0.601380 -0.196981

2 6 0 -2.910262 0.198233 0.423773

3 8 0 -4.603627 -0.286499 -1.197235

4 8 0 -4.257699 -1.762883 0.442550

5 6 0 -2.314449 -0.312377 1.713934

6 16 0 -1.597754 0.234761 -0.983283

7 6 0 -0.138490 0.762876 -0.193669

8 16 0 0.997771 -0.570841 0.181701

9 16 0 0.118785 2.395720 0.277270

10 6 0 2.635913 0.251759 0.054965

11 6 0 3.753396 -0.774761 -0.043782

12 6 0 5.126693 -0.104967 -0.115954

13 6 0 6.269186 -1.111114 -0.193819

14 1 0 -3.258981 1.223111 0.528189

15 1 0 -4.934782 -2.226311 -0.072700

16 1 0 -1.491386 0.330466 2.020698

17 1 0 -3.061156 -0.306367 2.510067

18 1 0 -1.936949 -1.328132 1.613913

19 1 0 2.616423 0.897442 -0.823029

20 1 0 2.760121 0.881548 0.932970

21 1 0 3.721620 -1.443260 0.822053

22 1 0 3.608185 -1.406121 -0.925522

23 1 0 5.161387 0.558680 -0.985376

24 1 0 5.260269 0.538131 0.759669

25 1 0 7.240605 -0.613530 -0.232196

26 1 0 6.274257 -1.776663 0.672826

27 1 0 6.189888 -1.737792 -1.085867

---------------------------------------------------------------------

Rotational constants (GHZ): 1.1959352 0.1992741 0.1857433

Leave Link 202 at Sat Aug 17 17:46:04 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1106.9935987428 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0552356364 Hartrees.

Nuclear repulsion after empirical dispersion term = 1106.9383631064 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

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Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2327

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.10D-11

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 112

GePol: Fraction of low-weight points (<1% of avg) = 4.81%

GePol: Cavity surface area = 306.733 Ang\*\*2

GePol: Cavity volume = 318.809 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0056572163 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1106.9327058901 Hartrees.

Leave Link 301 at Sat Aug 17 17:46:04 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.82D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:46:04 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:46:04 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999018 0.043909 0.003747 0.004489 Ang= 5.08 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.63221512350

Leave Link 401 at Sat Aug 17 17:46:05 2019, MaxMem= 1342177280 cpu: 7.7

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16244787.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.11D-15 for 2317.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.11D-15 for 2294 48.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.77D-15 for 2327.

Iteration 1 A^-1\*A deviation from orthogonality is 3.46D-12 for 900 719.

E= -1658.35598361268

DIIS: error= 2.22D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.35598361268 IErMin= 1 ErrMin= 2.22D-02

ErrMax= 2.22D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.49D-01 BMatP= 7.49D-01

IDIUse=3 WtCom= 7.78D-01 WtEn= 2.22D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Recover alternate guess density for next cycle.

RMSDP=2.75D-03 MaxDP=7.60D-02 OVMax= 0.00D+00

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.74D-03 CP: 9.89D-01

E= -1658.21629267639 Delta-E= 0.139690936296 Rises=F Damp=F

Switch densities from cycles 1 and 2 for lowest energy.

DIIS: error= 4.79D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 1 EnMin= -1658.35598361268 IErMin= 1 ErrMin= 2.22D-02

ErrMax= 4.79D-02 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.21D+00 BMatP= 7.49D-01

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.765D+00 0.235D+00

Coeff: 0.765D+00 0.235D+00

Gap= 0.117 Goal= None Shift= 0.000

Gap= 0.135 Goal= None Shift= 0.000

RMSDP=1.39D-02 MaxDP=5.42D-01 DE= 1.40D-01 OVMax= 1.82D-01

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.78D-03 CP: 9.91D-01 2.93D-01

E= -1658.61359217066 Delta-E= -0.397299494276 Rises=F Damp=F

DIIS: error= 1.85D-02 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.61359217066 IErMin= 3 ErrMin= 1.85D-02

ErrMax= 1.85D-02 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.05D-01 BMatP= 7.49D-01

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.473D-01 0.243D+00 0.709D+00

Coeff: 0.473D-01 0.243D+00 0.709D+00

Gap= 0.128 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=8.18D-04 MaxDP=5.08D-02 DE=-3.97D-01 OVMax= 5.36D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 5.06D-04 CP: 9.88D-01 4.51D-01 7.34D-01

E= -1658.66482230809 Delta-E= -0.051230137430 Rises=F Damp=F

DIIS: error= 8.01D-03 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.66482230809 IErMin= 4 ErrMin= 8.01D-03

ErrMax= 8.01D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 5.47D-02 BMatP= 3.05D-01

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.215D-01 0.107D+00 0.399D+00 0.516D+00

Coeff: -0.215D-01 0.107D+00 0.399D+00 0.516D+00

Gap= 0.124 Goal= None Shift= 0.000

Gap= 0.130 Goal= None Shift= 0.000

RMSDP=3.21D-04 MaxDP=1.80D-02 DE=-5.12D-02 OVMax= 3.28D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.99D-04 CP: 9.90D-01 4.62D-01 7.70D-01 5.25D-01

E= -1658.67354195533 Delta-E= -0.008719647241 Rises=F Damp=F

DIIS: error= 2.76D-03 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67354195533 IErMin= 5 ErrMin= 2.76D-03

ErrMax= 2.76D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 7.00D-03 BMatP= 5.47D-02

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.105D-01 0.202D-01 0.122D+00 0.300D+00 0.568D+00

Coeff: -0.105D-01 0.202D-01 0.122D+00 0.300D+00 0.568D+00

Gap= 0.125 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=1.34D-04 MaxDP=5.86D-03 DE=-8.72D-03 OVMax= 1.32D-02

Cycle 6 Pass 1 IDiag 1:

RMSU= 8.35D-05 CP: 9.89D-01 4.55D-01 7.75D-01 6.39D-01 5.78D-01

E= -1658.67488142260 Delta-E= -0.001339467262 Rises=F Damp=F

DIIS: error= 1.36D-03 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67488142260 IErMin= 6 ErrMin= 1.36D-03

ErrMax= 1.36D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 9.05D-04 BMatP= 7.00D-03

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.336D-02 0.291D-02 0.411D-01 0.140D+00 0.347D+00 0.472D+00

Coeff: -0.336D-02 0.291D-02 0.411D-01 0.140D+00 0.347D+00 0.472D+00

Gap= 0.126 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=3.75D-05 MaxDP=1.70D-03 DE=-1.34D-03 OVMax= 4.24D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.63D-05 CP: 9.89D-01 4.52D-01 7.78D-01 6.50D-01 6.64D-01

CP: 7.98D-01

E= -1658.67504926302 Delta-E= -0.000167840422 Rises=F Damp=F

DIIS: error= 2.03D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67504926302 IErMin= 7 ErrMin= 2.03D-04

ErrMax= 2.03D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 4.19D-05 BMatP= 9.05D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.728D-03-0.630D-03 0.555D-02 0.333D-01 0.103D+00 0.216D+00

Coeff-Com: 0.644D+00

Coeff: -0.728D-03-0.630D-03 0.555D-02 0.333D-01 0.103D+00 0.216D+00

Coeff: 0.644D+00

Gap= 0.126 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=1.44D-05 MaxDP=4.97D-04 DE=-1.68D-04 OVMax= 1.80D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.12D-05 CP: 9.89D-01 4.52D-01 7.77D-01 6.60D-01 6.94D-01

CP: 8.41D-01 9.05D-01

E= -1658.67505908584 Delta-E= -0.000009822826 Rises=F Damp=F

DIIS: error= 7.70D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67505908584 IErMin= 8 ErrMin= 7.70D-05

ErrMax= 7.70D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 6.88D-06 BMatP= 4.19D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.475D-04-0.753D-03-0.257D-02-0.636D-03 0.105D-01 0.489D-01

Coeff-Com: 0.307D+00 0.637D+00

Coeff: 0.475D-04-0.753D-03-0.257D-02-0.636D-03 0.105D-01 0.489D-01

Coeff: 0.307D+00 0.637D+00

Gap= 0.127 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=8.37D-06 MaxDP=3.07D-04 DE=-9.82D-06 OVMax= 1.33D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 4.40D-06 CP: 9.89D-01 4.52D-01 7.77D-01 6.64D-01 7.00D-01

CP: 9.01D-01 1.06D+00 1.05D+00

E= -1658.67506148414 Delta-E= -0.000002398295 Rises=F Damp=F

DIIS: error= 2.51D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67506148414 IErMin= 9 ErrMin= 2.51D-05

ErrMax= 2.51D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.04D-06 BMatP= 6.88D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.197D-03-0.129D-03-0.224D-02-0.812D-02-0.192D-01-0.315D-01

Coeff-Com: -0.535D-01 0.196D+00 0.918D+00

Coeff: 0.197D-03-0.129D-03-0.224D-02-0.812D-02-0.192D-01-0.315D-01

Coeff: -0.535D-01 0.196D+00 0.918D+00

Gap= 0.127 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=5.25D-06 MaxDP=2.22D-04 DE=-2.40D-06 OVMax= 7.22D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 2.04D-06 CP: 9.89D-01 4.52D-01 7.77D-01 6.67D-01 7.08D-01

CP: 9.35D-01 1.14D+00 1.28D+00 1.04D+00

E= -1658.67506211737 Delta-E= -0.000000633234 Rises=F Damp=F

DIIS: error= 1.34D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67506211737 IErMin=10 ErrMin= 1.34D-05

ErrMax= 1.34D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 4.75D-07 BMatP= 1.04D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.110D-03 0.958D-04-0.837D-03-0.490D-02-0.139D-01-0.289D-01

Coeff-Com: -0.921D-01-0.840D-02 0.554D+00 0.595D+00

Coeff: 0.110D-03 0.958D-04-0.837D-03-0.490D-02-0.139D-01-0.289D-01

Coeff: -0.921D-01-0.840D-02 0.554D+00 0.595D+00

Gap= 0.127 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=2.94D-06 MaxDP=1.30D-04 DE=-6.33D-07 OVMax= 5.18D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.01D-06 CP: 9.89D-01 4.51D-01 7.77D-01 6.69D-01 7.10D-01

CP: 9.51D-01 1.18D+00 1.40D+00 1.33D+00 7.77D-01

E= -1658.67506227148 Delta-E= -0.000000154103 Rises=F Damp=F

DIIS: error= 6.70D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67506227148 IErMin=11 ErrMin= 6.70D-06

ErrMax= 6.70D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 8.29D-08 BMatP= 4.75D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.397D-04 0.647D-04-0.128D-03-0.153D-02-0.475D-02-0.111D-01

Coeff-Com: -0.420D-01-0.360D-01 0.163D+00 0.340D+00 0.593D+00

Coeff: 0.397D-04 0.647D-04-0.128D-03-0.153D-02-0.475D-02-0.111D-01

Coeff: -0.420D-01-0.360D-01 0.163D+00 0.340D+00 0.593D+00

Gap= 0.127 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=7.15D-07 MaxDP=5.36D-05 DE=-1.54D-07 OVMax= 1.33D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 4.66D-07 CP: 9.89D-01 4.51D-01 7.77D-01 6.69D-01 7.11D-01

CP: 9.51D-01 1.18D+00 1.41D+00 1.35D+00 9.38D-01

CP: 6.98D-01

E= -1658.67506229679 Delta-E= -0.000000025311 Rises=F Damp=F

DIIS: error= 2.86D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.67506229679 IErMin=12 ErrMin= 2.86D-06

ErrMax= 2.86D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.68D-08 BMatP= 8.29D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.685D-05 0.137D-04 0.145D-03 0.354D-03 0.755D-03 0.745D-03

Coeff-Com: -0.134D-02-0.170D-01-0.457D-01 0.290D-01 0.347D+00 0.686D+00

Coeff: -0.685D-05 0.137D-04 0.145D-03 0.354D-03 0.755D-03 0.745D-03

Coeff: -0.134D-02-0.170D-01-0.457D-01 0.290D-01 0.347D+00 0.686D+00

Gap= 0.127 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=4.05D-07 MaxDP=2.10D-05 DE=-2.53D-08 OVMax= 4.09D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.80D-07 CP: 9.89D-01 4.51D-01 7.77D-01 6.69D-01 7.11D-01

CP: 9.53D-01 1.19D+00 1.43D+00 1.38D+00 9.95D-01

CP: 8.98D-01 8.44D-01

E= -1658.67506230232 Delta-E= -0.000000005531 Rises=F Damp=F

DIIS: error= 9.45D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1658.67506230232 IErMin=13 ErrMin= 9.45D-07

ErrMax= 9.45D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.14D-09 BMatP= 1.68D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.771D-05-0.313D-05 0.778D-04 0.358D-03 0.938D-03 0.174D-02

Coeff-Com: 0.475D-02-0.174D-02-0.373D-01-0.341D-01 0.792D-01 0.275D+00

Coeff-Com: 0.711D+00

Coeff: -0.771D-05-0.313D-05 0.778D-04 0.358D-03 0.938D-03 0.174D-02

Coeff: 0.475D-02-0.174D-02-0.373D-01-0.341D-01 0.792D-01 0.275D+00

Coeff: 0.711D+00

Gap= 0.127 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=1.08D-07 MaxDP=6.71D-06 DE=-5.53D-09 OVMax= 2.26D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 5.98D-08 CP: 9.89D-01 4.51D-01 7.77D-01 6.69D-01 7.11D-01

CP: 9.53D-01 1.19D+00 1.43D+00 1.39D+00 1.00D+00

CP: 9.47D-01 9.79D-01 8.97D-01

E= -1658.67506230275 Delta-E= -0.000000000429 Rises=F Damp=F

DIIS: error= 3.14D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1658.67506230275 IErMin=14 ErrMin= 3.14D-07

ErrMax= 3.14D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.86D-10 BMatP= 1.14D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.211D-05-0.267D-05 0.992D-05 0.909D-04 0.253D-03 0.590D-03

Coeff-Com: 0.218D-02 0.178D-02-0.938D-02-0.199D-01-0.121D-01 0.142D-01

Coeff-Com: 0.289D+00 0.733D+00

Coeff: -0.211D-05-0.267D-05 0.992D-05 0.909D-04 0.253D-03 0.590D-03

Coeff: 0.218D-02 0.178D-02-0.938D-02-0.199D-01-0.121D-01 0.142D-01

Coeff: 0.289D+00 0.733D+00

Gap= 0.127 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=4.91D-08 MaxDP=3.62D-06 DE=-4.29D-10 OVMax= 5.19D-06

Cycle 15 Pass 1 IDiag 1:

RMSU= 2.53D-08 CP: 9.89D-01 4.51D-01 7.77D-01 6.69D-01 7.11D-01

CP: 9.53D-01 1.19D+00 1.43D+00 1.39D+00 1.01D+00

CP: 9.62D-01 1.01D+00 1.06D+00 8.82D-01

E= -1658.67506230281 Delta-E= -0.000000000065 Rises=F Damp=F

DIIS: error= 1.11D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1658.67506230281 IErMin=15 ErrMin= 1.11D-07

ErrMax= 1.11D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.45D-11 BMatP= 1.86D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.504D-06-0.411D-06-0.112D-04-0.312D-04-0.779D-04-0.996D-04

Coeff-Com: -0.113D-03 0.936D-03 0.404D-02-0.126D-02-0.186D-01-0.531D-01

Coeff-Com: -0.180D-01 0.338D+00 0.748D+00

Coeff: 0.504D-06-0.411D-06-0.112D-04-0.312D-04-0.779D-04-0.996D-04

Coeff: -0.113D-03 0.936D-03 0.404D-02-0.126D-02-0.186D-01-0.531D-01

Coeff: -0.180D-01 0.338D+00 0.748D+00

Gap= 0.127 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=2.01D-08 MaxDP=1.47D-06 DE=-6.50D-11 OVMax= 4.81D-06

Cycle 16 Pass 1 IDiag 1:

RMSU= 8.67D-09 CP: 9.89D-01 4.51D-01 7.77D-01 6.69D-01 7.11D-01

CP: 9.53D-01 1.19D+00 1.43D+00 1.39D+00 1.01D+00

CP: 9.68D-01 1.03D+00 1.10D+00 1.07D+00 8.49D-01

E= -1658.67506230280 Delta-E= 0.000000000014 Rises=F Damp=F

DIIS: error= 2.88D-08 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=15 EnMin= -1658.67506230281 IErMin=16 ErrMin= 2.88D-08

ErrMax= 2.88D-08 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.65D-12 BMatP= 3.45D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.372D-06 0.333D-07-0.450D-05-0.176D-04-0.457D-04-0.794D-04

Coeff-Com: -0.225D-03 0.112D-03 0.216D-02 0.128D-02-0.480D-02-0.203D-01

Coeff-Com: -0.322D-01 0.454D-01 0.274D+00 0.735D+00

Coeff: 0.372D-06 0.333D-07-0.450D-05-0.176D-04-0.457D-04-0.794D-04

Coeff: -0.225D-03 0.112D-03 0.216D-02 0.128D-02-0.480D-02-0.203D-01

Coeff: -0.322D-01 0.454D-01 0.274D+00 0.735D+00

Gap= 0.127 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=5.64D-09 MaxDP=3.13D-07 DE= 1.36D-11 OVMax= 5.84D-07

Error on total polarization charges = 0.04166

SCF Done: E(UB3LYP) = -1658.67506230 A.U. after 16 cycles

NFock= 16 Conv=0.56D-08 -V/T= 2.0020

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7551 S= 0.5025

<L.S>= 0.000000000000E+00

KE= 1.655367607942D+03 PE=-6.156816003989D+03 EE= 1.735840627854D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.55

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7551, after 0.7500

Leave Link 502 at Sat Aug 17 17:46:39 2019, MaxMem= 1342177280 cpu: 401.7

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 345

Leave Link 701 at Sat Aug 17 17:46:40 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:46:40 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:46:43 2019, MaxMem= 1342177280 cpu: 38.7

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.21520748D+00-2.93664778D+00 9.02754665D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.009371982 -0.004857593 0.011738875

2 6 0.001590890 0.001047346 -0.002820614

3 8 -0.009449107 0.006711226 -0.011243146

4 8 0.000803054 -0.001983235 0.001390446

5 6 -0.001815711 -0.001025718 0.000976880

6 16 -0.000877575 -0.001679809 -0.001142017

7 6 0.001121842 0.000690997 -0.001403678

8 16 -0.000034176 0.000780776 -0.001223204

9 16 0.000492354 0.001391826 0.002590796

10 6 -0.001437064 -0.000727564 0.000249688

11 6 0.000623168 -0.000274364 0.000331912

12 6 0.000072979 -0.000236094 0.000356955

13 6 0.000744387 -0.000262964 -0.000242758

14 1 -0.000008023 0.002130754 0.000159728

15 1 -0.002778148 -0.002466996 -0.001195850

16 1 0.000974621 0.000719806 0.000539923

17 1 -0.001428034 0.000126990 0.001181027

18 1 0.000806503 -0.001192545 -0.000636395

19 1 -0.000654638 0.000331663 -0.000935818

20 1 0.001340352 0.001385876 0.001122437

21 1 0.000283353 -0.001147051 0.001219638

22 1 -0.000414396 0.000065579 -0.001157525

23 1 -0.000156150 0.000890750 -0.001206854

24 1 0.000257094 0.000113633 0.001231757

25 1 0.001117427 0.000823599 0.000235043

26 1 -0.000052671 -0.000947844 0.001131137

27 1 -0.000494313 -0.000409043 -0.001248382

-------------------------------------------------------------------

Cartesian Forces: Max 0.011738875 RMS 0.002733759

Leave Link 716 at Sat Aug 17 17:46:43 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.016018805 RMS 0.001910731

Search for a local minimum.

Step number 36 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .19107D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 1 3 4 5 6

2 8 9 10 11

12 13 14 15 16

17 18 20 21 22

23 24 19 26 28

30 31 27 34 35

36 33

DE= 1.92D-03 DEPred=-4.65D-04 R=-4.12D+00

Trust test=-4.12D+00 RLast= 1.20D+00 DXMaxT set to 5.00D-02

ITU= -1 -1 -1 0 -1 0 0 -1 -1 0 0 -1 0 0 -1 1 -1 1 -1 1

ITU= 1 -1 1 -1 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.92797.

Iteration 1 RMS(Cart)= 0.18694543 RMS(Int)= 0.04493219

Iteration 2 RMS(Cart)= 0.07267519 RMS(Int)= 0.00450514

Iteration 3 RMS(Cart)= 0.00569309 RMS(Int)= 0.00003241

Iteration 4 RMS(Cart)= 0.00003801 RMS(Int)= 0.00002229

Iteration 5 RMS(Cart)= 0.00000000 RMS(Int)= 0.00002229

ITry= 1 IFail=0 DXMaxC= 9.44D-01 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=T

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83192 0.00227 0.00540 0.00000 0.00540 2.83732

R2 2.27225 0.01602 0.01459 0.00000 0.01459 2.28684

R3 2.54718 0.00453 0.00577 0.00000 0.00577 2.55295

R4 2.85357 0.00171 0.01229 0.00000 0.01229 2.86585

R5 3.63684 0.00153 -0.03654 0.00000 -0.03654 3.60029

R6 2.05527 0.00198 0.00240 0.00000 0.00240 2.05768

R7 1.83088 0.00358 0.00559 0.00000 0.00559 1.83647

R8 2.05693 0.00133 0.00402 0.00000 0.00402 2.06094

R9 2.06269 0.00181 0.00567 0.00000 0.00567 2.06836

R10 2.05648 0.00152 0.00353 0.00000 0.00353 2.06001

R11 3.29043 0.00337 0.02853 0.00000 0.02853 3.31896

R12 3.38614 0.00057 -0.00173 0.00000 -0.00173 3.38442

R13 3.24800 0.00247 0.00570 0.00000 0.00570 3.25370

R14 3.47229 0.00087 0.00293 0.00000 0.00293 3.47521

R15 2.87354 0.00233 0.00706 0.00000 0.00706 2.88060

R16 2.05985 0.00088 0.00382 0.00000 0.00382 2.06367

R17 2.05534 0.00172 0.00455 0.00000 0.00455 2.05988

R18 2.89059 0.00127 0.00334 0.00000 0.00334 2.89393

R19 2.06800 0.00166 0.00408 0.00000 0.00408 2.07208

R20 2.06765 0.00107 0.00312 0.00000 0.00312 2.07076

R21 2.88063 0.00156 0.00509 0.00000 0.00509 2.88572

R22 2.06796 0.00145 0.00374 0.00000 0.00374 2.07169

R23 2.06848 0.00117 0.00306 0.00000 0.00306 2.07154

R24 2.06380 0.00137 0.00362 0.00000 0.00362 2.06742

R25 2.06496 0.00147 0.00397 0.00000 0.00397 2.06893

R26 2.06557 0.00135 0.00321 0.00000 0.00321 2.06878

A1 2.17202 0.00051 0.00515 0.00000 0.00516 2.17718

A2 1.97781 0.00060 -0.00223 0.00000 -0.00222 1.97559

A3 2.13216 -0.00105 -0.00220 0.00000 -0.00220 2.12996

A4 2.05378 -0.00360 -0.02981 0.00000 -0.02978 2.02400

A5 1.78253 0.00277 0.05199 0.00000 0.05197 1.83450

A6 1.88194 0.00089 -0.00964 0.00000 -0.00961 1.87233

A7 1.94119 0.00086 0.00532 0.00000 0.00530 1.94649

A8 1.94242 0.00061 -0.00227 0.00000 -0.00224 1.94018

A9 1.84520 -0.00124 -0.01166 0.00000 -0.01167 1.83353

A10 1.86037 0.00266 0.01300 0.00000 0.01300 1.87337

A11 1.91712 0.00005 -0.00490 0.00000 -0.00490 1.91222

A12 1.92985 -0.00043 -0.00176 0.00000 -0.00176 1.92809

A13 1.95408 -0.00015 -0.00145 0.00000 -0.00145 1.95262

A14 1.88438 0.00010 -0.00069 0.00000 -0.00069 1.88369

A15 1.89109 0.00000 0.00247 0.00000 0.00247 1.89356

A16 1.88544 0.00045 0.00656 0.00000 0.00656 1.89200

A17 1.81910 0.00108 -0.02343 0.00000 -0.02343 1.79568

A18 1.98306 -0.00137 -0.01116 0.00000 -0.01103 1.97203

A19 2.13867 0.00210 0.00328 0.00000 0.00342 2.14209

A20 2.15891 -0.00089 -0.00493 0.00000 -0.00480 2.15411

A21 1.79022 0.00474 0.00400 0.00000 0.00400 1.79422

A22 1.93632 -0.00108 -0.00928 0.00000 -0.00928 1.92703

A23 1.88053 -0.00045 -0.00448 0.00000 -0.00447 1.87606

A24 1.88111 0.00157 0.01298 0.00000 0.01298 1.89410

A25 1.93983 0.00081 -0.00064 0.00000 -0.00064 1.93919

A26 1.93841 -0.00067 0.00025 0.00000 0.00025 1.93866

A27 1.88523 -0.00012 0.00163 0.00000 0.00163 1.88686

A28 1.94684 0.00132 0.00646 0.00000 0.00646 1.95330

A29 1.91735 -0.00001 -0.00001 0.00000 -0.00001 1.91735

A30 1.92233 -0.00088 -0.00678 0.00000 -0.00678 1.91555

A31 1.90804 -0.00070 -0.00161 0.00000 -0.00161 1.90643

A32 1.91113 -0.00017 -0.00156 0.00000 -0.00156 1.90957

A33 1.85590 0.00040 0.00333 0.00000 0.00333 1.85922

A34 1.96739 0.00032 -0.00083 0.00000 -0.00083 1.96656

A35 1.90869 -0.00031 -0.00226 0.00000 -0.00226 1.90643

A36 1.90613 0.00002 0.00142 0.00000 0.00142 1.90755

A37 1.91340 -0.00004 -0.00080 0.00000 -0.00080 1.91260

A38 1.91473 -0.00025 -0.00162 0.00000 -0.00162 1.91311

A39 1.84978 0.00026 0.00442 0.00000 0.00442 1.85420

A40 1.94736 -0.00017 -0.00170 0.00000 -0.00170 1.94566

A41 1.94441 -0.00010 -0.00190 0.00000 -0.00190 1.94251

A42 1.94522 -0.00051 -0.00189 0.00000 -0.00189 1.94333

A43 1.87679 0.00013 -0.00031 0.00000 -0.00031 1.87648

A44 1.87242 0.00040 0.00430 0.00000 0.00430 1.87671

A45 1.87381 0.00031 0.00188 0.00000 0.00189 1.87569

D1 3.09881 -0.00197 -0.41449 0.00000 -0.41451 2.68430

D2 -1.05403 -0.00088 -0.38664 0.00000 -0.38663 -1.44066

D3 0.88532 -0.00075 -0.38081 0.00000 -0.38079 0.50453

D4 -0.09441 -0.00079 -0.39486 0.00000 -0.39488 -0.48928

D5 2.03593 0.00030 -0.36700 0.00000 -0.36699 1.66894

D6 -2.30790 0.00043 -0.36117 0.00000 -0.36116 -2.66905

D7 -3.06939 -0.00104 -0.03524 0.00000 -0.03524 -3.10463

D8 0.02191 0.00016 -0.01596 0.00000 -0.01596 0.00595

D9 3.08696 0.00106 0.06967 0.00000 0.06968 -3.12654

D10 -1.11824 0.00095 0.06467 0.00000 0.06468 -1.05356

D11 0.98514 0.00112 0.07082 0.00000 0.07082 1.05597

D12 1.04020 -0.00077 0.01771 0.00000 0.01770 1.05790

D13 3.11818 -0.00088 0.01271 0.00000 0.01271 3.13089

D14 -1.06163 -0.00071 0.01885 0.00000 0.01885 -1.04278

D15 -1.01234 -0.00017 0.03033 0.00000 0.03033 -0.98201

D16 1.06565 -0.00028 0.02534 0.00000 0.02533 1.09098

D17 -3.11416 -0.00011 0.03148 0.00000 0.03148 -3.08268

D18 -2.88227 0.00109 -0.24965 0.00000 -0.24962 -3.13190

D19 -0.67662 -0.00101 -0.24840 0.00000 -0.24843 -0.92505

D20 1.43401 -0.00055 -0.25542 0.00000 -0.25542 1.17859

D21 1.75962 0.00007 0.07599 0.00000 0.07599 1.83561

D22 -1.30787 0.00246 0.18124 0.00000 0.18124 -1.12664

D23 2.59606 0.00083 -0.03941 0.00000 -0.03939 2.55667

D24 -0.62061 -0.00145 -0.14506 0.00000 -0.14508 -0.76569

D25 -2.86568 -0.00077 -0.14080 0.00000 -0.14079 -3.00648

D26 -0.73864 -0.00072 -0.15005 0.00000 -0.15005 -0.88869

D27 1.29182 -0.00029 -0.14375 0.00000 -0.14375 1.14806

D28 -3.11761 -0.00045 0.00695 0.00000 0.00695 -3.11067

D29 -0.99901 -0.00047 0.00922 0.00000 0.00922 -0.98979

D30 1.03963 -0.00051 0.00927 0.00000 0.00927 1.04890

D31 1.07356 0.00030 0.01908 0.00000 0.01908 1.09264

D32 -3.09102 0.00028 0.02135 0.00000 0.02135 -3.06967

D33 -1.05238 0.00024 0.02141 0.00000 0.02141 -1.03098

D34 -1.02580 0.00036 0.01728 0.00000 0.01728 -1.00852

D35 1.09281 0.00034 0.01955 0.00000 0.01955 1.11236

D36 3.13145 0.00030 0.01960 0.00000 0.01960 -3.13213

D37 3.12599 0.00028 0.03167 0.00000 0.03167 -3.12553

D38 -1.02404 0.00023 0.02847 0.00000 0.02847 -0.99557

D39 0.99297 0.00037 0.03329 0.00000 0.03329 1.02626

D40 1.00198 -0.00009 0.02852 0.00000 0.02852 1.03051

D41 3.13514 -0.00014 0.02533 0.00000 0.02533 -3.12272

D42 -1.13104 0.00000 0.03014 0.00000 0.03014 -1.10089

D43 -1.02479 -0.00007 0.02632 0.00000 0.02632 -0.99847

D44 1.10837 -0.00013 0.02312 0.00000 0.02312 1.13149

D45 3.12537 0.00002 0.02794 0.00000 0.02794 -3.12987

D46 -3.12940 -0.00010 -0.01212 0.00000 -0.01212 -3.14152

D47 -1.03158 -0.00012 -0.01497 0.00000 -0.01497 -1.04655

D48 1.06098 -0.00014 -0.01514 0.00000 -0.01514 1.04584

D49 1.02328 0.00011 -0.00809 0.00000 -0.00809 1.01519

D50 3.12110 0.00008 -0.01094 0.00000 -0.01094 3.11016

D51 -1.06952 0.00006 -0.01111 0.00000 -0.01111 -1.08063

D52 -1.00123 -0.00003 -0.01203 0.00000 -0.01203 -1.01326

D53 1.09659 -0.00006 -0.01488 0.00000 -0.01488 1.08171

D54 -3.09403 -0.00008 -0.01505 0.00000 -0.01505 -3.10908

Item Value Threshold Converged?

Maximum Force 0.016019 0.000450 NO

RMS Force 0.001911 0.000300 NO

Maximum Displacement 0.943750 0.001800 NO

RMS Displacement 0.237925 0.001200 NO

Predicted change in Energy=-1.636408D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:46:44 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.101426 -0.383935 -0.216720

2 6 0 -2.840234 0.062761 0.464601

3 8 0 -4.882658 0.353445 -0.773848

4 8 0 -4.276312 -1.723208 -0.187406

5 6 0 -2.336945 -0.830574 1.581991

6 16 0 -1.553875 0.228635 -0.930937

7 6 0 -0.107553 0.734224 -0.072341

8 16 0 1.099725 -0.577726 0.097331

9 16 0 0.005301 2.239724 0.755466

10 6 0 2.698795 0.326529 0.012291

11 6 0 3.862461 -0.656074 -0.051003

12 6 0 5.215269 0.061084 -0.078993

13 6 0 6.393106 -0.907002 -0.165066

14 1 0 -3.006335 1.079078 0.818383

15 1 0 -5.092528 -1.919445 -0.677013

16 1 0 -1.430169 -0.402814 2.011170

17 1 0 -3.083993 -0.905061 2.378460

18 1 0 -2.110559 -1.836210 1.227326

19 1 0 2.670533 0.960397 -0.876518

20 1 0 2.778287 0.972476 0.886721

21 1 0 3.828592 -1.329641 0.813560

22 1 0 3.766312 -1.287100 -0.941700

23 1 0 5.241771 0.748833 -0.932315

24 1 0 5.314489 0.682412 0.818666

25 1 0 7.348670 -0.374601 -0.183763

26 1 0 6.411877 -1.587646 0.692269

27 1 0 6.339558 -1.520196 -1.070388

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.501447 0.000000

3 O 1.210143 2.406190 0.000000

4 O 1.350961 2.382671 2.241441 0.000000

5 C 2.558953 1.516545 3.665042 2.772852 0.000000

6 S 2.715762 1.905192 3.334824 3.431354 2.837239

7 C 4.149957 2.864736 4.841357 4.840533 3.186784

8 S 5.214226 4.008539 6.116775 5.504087 3.752179

9 S 4.969300 3.594557 5.457930 5.909826 3.949176

10 C 6.841068 5.563721 7.622150 7.272786 5.400141

11 C 7.970258 6.760820 8.832822 8.209568 6.413248

12 C 9.328334 8.073823 10.126027 9.658445 7.783948

13 C 10.507685 9.305454 11.362315 10.700615 8.903473

14 H 2.100254 1.088876 2.565605 3.236859 2.162858

15 H 1.884660 3.210180 2.284612 0.971819 3.725852

16 H 3.478428 2.144043 4.499771 3.831149 1.090603

17 H 2.835789 2.158461 3.841364 2.945277 1.094528

18 H 2.856207 2.172617 4.060027 2.589348 1.090110

19 H 6.935559 5.742203 7.578234 7.478988 5.858897

20 H 7.098442 5.707323 7.863255 7.628095 5.468088

21 H 8.052392 6.821568 9.013242 8.175959 6.233249

22 H 7.952521 6.888124 8.804785 8.089681 6.620209

23 H 9.438780 8.230484 10.133386 9.862037 8.139607

24 H 9.532501 8.185893 10.325994 9.938947 7.836851

25 H 11.450147 10.218875 12.267177 11.702947 9.855807

26 H 10.620956 9.400916 11.553521 10.725185 8.826474

27 H 10.537267 9.440896 11.381415 10.654463 9.099033

6 7 8 9 10

6 S 0.000000

7 C 1.756318 0.000000

8 S 2.957895 1.790955 0.000000

9 S 3.052779 1.721781 3.093369 0.000000

10 C 4.357116 2.837070 1.839004 3.386375 0.000000

11 C 5.558209 4.206471 2.767824 4.890166 1.524347

12 C 6.824602 5.365221 4.168557 5.708463 2.532081

13 C 8.064163 6.705280 5.310099 7.180063 3.898844

14 H 2.427553 3.052090 4.486050 3.228159 5.810734

15 H 4.147383 5.679574 6.383088 6.733390 8.137828

16 H 3.011648 2.717201 3.177064 3.258892 4.644976

17 H 3.818198 4.189615 4.776421 4.697608 6.368376

18 H 3.038351 3.508318 3.628580 4.616573 5.411435

19 H 4.287664 2.900968 2.404505 3.376908 1.092048

20 H 4.756554 3.050350 2.417403 3.051655 1.090044

21 H 5.868769 4.531843 2.919773 5.230802 2.159021

22 H 5.531903 4.455150 2.948471 5.428080 2.157194

23 H 6.815528 5.418029 4.469505 5.700173 2.745423

24 H 7.102215 5.495009 4.457860 5.533235 2.760209

25 H 8.954187 7.539043 6.258561 7.851236 4.706523

26 H 8.329879 6.962663 5.439931 7.463040 4.232424

27 H 8.086047 6.902445 5.450474 7.589042 4.223475

11 12 13 14 15

11 C 0.000000

12 C 1.531401 0.000000

13 C 2.545611 1.527056 0.000000

14 H 7.137713 8.332849 9.657182 0.000000

15 H 9.065309 10.513363 11.541530 3.947094 0.000000

16 H 5.685827 6.981821 8.135959 2.470435 4.789506

17 H 7.363254 8.709205 9.812488 2.525209 3.794615

18 H 6.221239 7.679449 8.666861 3.077101 3.539149

19 H 2.171440 2.814337 4.225032 5.925673 8.282415

20 H 2.169547 2.775269 4.207803 5.786008 8.529842

21 H 1.096498 2.157230 2.777240 7.246943 9.063998

22 H 1.095801 2.159014 2.765444 7.386842 8.885323

23 H 2.157075 1.096293 2.157784 8.438321 10.676265

24 H 2.157836 1.096214 2.158096 8.330274 10.831100

25 H 3.500072 2.179954 1.094031 10.504457 12.546443

26 H 2.814214 2.178308 1.094829 9.789282 11.590356

27 H 2.814581 2.178839 1.094752 9.882784 11.445818

16 17 18 19 20

16 H 0.000000

17 H 1.767000 0.000000

18 H 1.769735 1.771926 0.000000

19 H 5.197388 6.869453 5.925032 0.000000

20 H 4.568031 6.333779 5.648499 1.766570 0.000000

21 H 5.472462 7.100212 5.975059 3.072742 2.531449

22 H 6.041921 7.622079 6.288386 2.501244 3.070016

23 H 7.382762 9.111254 8.087228 2.580531 3.070450

24 H 6.934710 8.688356 7.851229 3.153004 2.553643

25 H 9.049118 10.755781 9.674941 4.913970 4.883539

26 H 8.039963 9.668542 8.542832 4.790749 4.449158

27 H 8.432864 10.053669 8.762639 4.433134 4.767215

21 22 23 24 25

21 H 0.000000

22 H 1.756880 0.000000

23 H 3.060263 2.514377 0.000000

24 H 2.501255 3.061817 1.753748 0.000000

25 H 3.781230 3.773647 2.502291 2.502006 0.000000

26 H 2.598969 3.123972 3.076939 2.524559 1.765358

27 H 3.144920 2.586985 2.524419 3.077462 1.765445

26 27

26 H 0.000000

27 H 1.765429 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 4.54D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.113171 -0.437080 -0.154381

2 6 0 -2.846461 0.111446 0.436302

3 8 0 -4.898566 0.202252 -0.816842

4 8 0 -4.288253 -1.753888 0.091503

5 6 0 -2.334601 -0.591178 1.678972

6 16 0 -1.571177 0.048462 -0.977713

7 6 0 -0.117916 0.683352 -0.222993

8 16 0 1.090247 -0.586106 0.146250

9 16 0 0.001999 2.302289 0.350763

10 6 0 2.688884 0.290111 -0.095696

11 6 0 3.851692 -0.691725 -0.009049

12 6 0 5.204467 0.009412 -0.162656

13 6 0 6.381269 -0.961786 -0.100938

14 1 0 -3.009418 1.171722 0.623150

15 1 0 -5.108396 -2.025073 -0.353757

16 1 0 -1.424306 -0.101362 2.026618

17 1 0 -3.075323 -0.535293 2.482838

18 1 0 -2.111366 -1.641150 1.489063

19 1 0 2.653767 0.772688 -1.074704

20 1 0 2.775530 1.068263 0.662702

21 1 0 3.824475 -1.217286 0.952904

22 1 0 3.748266 -1.457742 -0.785774

23 1 0 5.224412 0.550791 -1.115740

24 1 0 5.311017 0.766974 0.622477

25 1 0 7.336828 -0.440866 -0.212537

26 1 0 6.406630 -1.495579 0.854611

27 1 0 6.320333 -1.712626 -0.895299

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3186265 0.1924730 0.1802673

Leave Link 202 at Sat Aug 17 17:46:44 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1101.7742678567 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0549369236 Hartrees.

Nuclear repulsion after empirical dispersion term = 1101.7193309331 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2319

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.21D-08

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 104

GePol: Fraction of low-weight points (<1% of avg) = 4.48%

GePol: Cavity surface area = 309.502 Ang\*\*2

GePol: Cavity volume = 320.277 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057959114 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1101.7135350218 Hartrees.

Leave Link 301 at Sat Aug 17 17:46:44 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:46:44 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:46:44 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Lowest energy guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999999 0.000981 -0.000033 0.000215 Ang= 0.12 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999609 -0.027749 -0.000895 -0.003267 Ang= -3.20 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 7.20D-02

Max alpha theta= 15.387 degrees.

Max beta theta= 15.691 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 17:46:44 2019, MaxMem= 1342177280 cpu: 4.3

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16133283.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.11D-15 for 2310.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.57D-15 for 2286 48.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.22D-15 for 2310.

Iteration 1 A^-1\*A deviation from orthogonality is 5.08D-12 for 1580 1526.

E= -1658.67692543228

DIIS: error= 7.34D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67692543228 IErMin= 1 ErrMin= 7.34D-04

ErrMax= 7.34D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.12D-04 BMatP= 3.12D-04

IDIUse=3 WtCom= 9.93D-01 WtEn= 7.34D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 88.658 Goal= None Shift= 0.000

Gap= 88.653 Goal= None Shift= 0.000

RMSDP=3.96D-05 MaxDP=2.33D-03 OVMax= 3.41D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.95D-05 CP: 1.00D+00

E= -1658.67690361595 Delta-E= 0.000021816336 Rises=F Damp=F

DIIS: error= 7.24D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 1 EnMin= -1658.67692543228 IErMin= 2 ErrMin= 7.24D-04

ErrMax= 7.24D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.19D-04 BMatP= 3.12D-04

IDIUse=3 WtCom= 2.71D-01 WtEn= 7.29D-01

Coeff-Com: 0.574D+00 0.426D+00

Coeff-En: 0.577D+00 0.423D+00

Coeff: 0.576D+00 0.424D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.86D-05 MaxDP=1.83D-03 DE= 2.18D-05 OVMax= 2.31D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.88D-05 CP: 1.00D+00 4.58D-01

E= -1658.67698959378 Delta-E= -0.000085977832 Rises=F Damp=F

DIIS: error= 2.48D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67698959378 IErMin= 3 ErrMin= 2.48D-04

ErrMax= 2.48D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.94D-05 BMatP= 3.12D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.48D-03

Coeff-Com: 0.846D-01 0.220D+00 0.695D+00

Coeff-En: 0.000D+00 0.415D-01 0.958D+00

Coeff: 0.844D-01 0.220D+00 0.696D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=9.04D-06 MaxDP=4.39D-04 DE=-8.60D-05 OVMax= 9.52D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 6.17D-06 CP: 1.00D+00 5.65D-01 7.30D-01

E= -1658.67699435891 Delta-E= -0.000004765133 Rises=F Damp=F

DIIS: error= 1.64D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67699435891 IErMin= 4 ErrMin= 1.64D-04

ErrMax= 1.64D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.25D-05 BMatP= 3.94D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.64D-03

Coeff-Com: -0.856D-02 0.997D-01 0.462D+00 0.447D+00

Coeff-En: 0.000D+00 0.000D+00 0.240D+00 0.760D+00

Coeff: -0.855D-02 0.995D-01 0.461D+00 0.448D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.82D-06 MaxDP=1.96D-04 DE=-4.77D-06 OVMax= 3.77D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.30D-06 CP: 1.00D+00 5.65D-01 8.24D-01 4.92D-01

E= -1658.67699657323 Delta-E= -0.000002214317 Rises=F Damp=F

DIIS: error= 1.87D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67699657323 IErMin= 5 ErrMin= 1.87D-05

ErrMax= 1.87D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.68D-07 BMatP= 1.25D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.858D-02 0.370D-01 0.186D+00 0.219D+00 0.567D+00

Coeff: -0.858D-02 0.370D-01 0.186D+00 0.219D+00 0.567D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.82D-07 MaxDP=4.26D-05 DE=-2.21D-06 OVMax= 5.65D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 5.35D-07 CP: 1.00D+00 5.67D-01 8.26D-01 5.06D-01 6.89D-01

E= -1658.67699661691 Delta-E= -0.000000043681 Rises=F Damp=F

DIIS: error= 3.21D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67699661691 IErMin= 6 ErrMin= 3.21D-06

ErrMax= 3.21D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.71D-08 BMatP= 2.68D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.278D-02 0.739D-02 0.406D-01 0.566D-01 0.251D+00 0.647D+00

Coeff: -0.278D-02 0.739D-02 0.406D-01 0.566D-01 0.251D+00 0.647D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.40D-07 MaxDP=1.29D-05 DE=-4.37D-08 OVMax= 2.32D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.79D-07 CP: 1.00D+00 5.67D-01 8.24D-01 5.15D-01 7.68D-01

CP: 8.21D-01

E= -1658.67699662059 Delta-E= -0.000000003683 Rises=F Damp=F

DIIS: error= 1.25D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67699662059 IErMin= 7 ErrMin= 1.25D-06

ErrMax= 1.25D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.48D-09 BMatP= 1.71D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.375D-03-0.662D-04 0.117D-02 0.459D-02 0.541D-01 0.273D+00

Coeff-Com: 0.668D+00

Coeff: -0.375D-03-0.662D-04 0.117D-02 0.459D-02 0.541D-01 0.273D+00

Coeff: 0.668D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=9.80D-08 MaxDP=4.44D-06 DE=-3.68D-09 OVMax= 6.59D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 7.42D-08 CP: 1.00D+00 5.67D-01 8.26D-01 5.17D-01 7.76D-01

CP: 8.94D-01 7.78D-01

E= -1658.67699662097 Delta-E= -0.000000000375 Rises=F Damp=F

DIIS: error= 4.37D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67699662097 IErMin= 8 ErrMin= 4.37D-07

ErrMax= 4.37D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.51D-10 BMatP= 1.48D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.171D-03-0.988D-03-0.479D-02-0.536D-02-0.750D-02 0.450D-01

Coeff-Com: 0.329D+00 0.644D+00

Coeff: 0.171D-03-0.988D-03-0.479D-02-0.536D-02-0.750D-02 0.450D-01

Coeff: 0.329D+00 0.644D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.34D-08 MaxDP=1.29D-06 DE=-3.75D-10 OVMax= 6.08D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.25D-08 CP: 1.00D+00 5.67D-01 8.26D-01 5.17D-01 7.86D-01

CP: 9.23D-01 9.33D-01 8.39D-01

E= -1658.67699662102 Delta-E= -0.000000000055 Rises=F Damp=F

DIIS: error= 7.02D-08 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67699662102 IErMin= 9 ErrMin= 7.02D-08

ErrMax= 7.02D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.43D-11 BMatP= 2.51D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.786D-04-0.301D-03-0.154D-02-0.196D-02-0.665D-02-0.112D-01

Coeff-Com: 0.243D-01 0.188D+00 0.809D+00

Coeff: 0.786D-04-0.301D-03-0.154D-02-0.196D-02-0.665D-02-0.112D-01

Coeff: 0.243D-01 0.188D+00 0.809D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.77D-08 MaxDP=6.47D-07 DE=-5.50D-11 OVMax= 2.36D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 9.19D-09 CP: 1.00D+00 5.67D-01 8.26D-01 5.18D-01 7.89D-01

CP: 9.33D-01 9.78D-01 9.69D-01 1.16D+00

E= -1658.67699662109 Delta-E= -0.000000000073 Rises=F Damp=F

DIIS: error= 5.42D-08 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67699662109 IErMin=10 ErrMin= 5.42D-08

ErrMax= 5.42D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.05D-12 BMatP= 1.43D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.108D-04 0.210D-04 0.785D-04-0.230D-04-0.205D-02-0.140D-01

Coeff-Com: -0.511D-01-0.132D-01 0.409D+00 0.671D+00

Coeff: 0.108D-04 0.210D-04 0.785D-04-0.230D-04-0.205D-02-0.140D-01

Coeff: -0.511D-01-0.132D-01 0.409D+00 0.671D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=7.77D-09 MaxDP=4.12D-07 DE=-7.32D-11 OVMax= 9.92D-07

Error on total polarization charges = 0.04168

SCF Done: E(UB3LYP) = -1658.67699662 A.U. after 10 cycles

NFock= 10 Conv=0.78D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655245009590D+03 PE=-6.146198620000D+03 EE= 1.730563078767D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.64

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:47:07 2019, MaxMem= 1342177280 cpu: 258.4

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 336

Leave Link 701 at Sat Aug 17 17:47:08 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:47:08 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:47:11 2019, MaxMem= 1342177280 cpu: 38.6

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.36870813D+00-2.93339585D+00 5.93547589D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000884896 -0.000644029 0.000904697

2 6 -0.000158539 -0.000389850 0.000115987

3 8 -0.000924311 0.000850576 -0.000737158

4 8 0.000218060 -0.000175503 0.000005050

5 6 0.000086551 -0.000073912 0.000004061

6 16 0.000109528 0.000290785 -0.000190960

7 6 -0.000153403 0.000014614 -0.000140092

8 16 0.000275551 -0.000121992 0.000025306

9 16 -0.000080228 0.000008557 0.000227263

10 6 -0.000269603 -0.000051961 0.000041076

11 6 0.000014699 -0.000099518 -0.000028319

12 6 -0.000048954 0.000057842 -0.000067907

13 6 0.000060208 -0.000066109 0.000000302

14 1 0.000015803 0.000205808 -0.000054448

15 1 -0.000230795 0.000023903 -0.000156045

16 1 0.000204447 0.000039129 0.000098954

17 1 -0.000086389 0.000035648 0.000089957

18 1 0.000010475 -0.000071618 -0.000110475

19 1 0.000097083 0.000149838 -0.000082579

20 1 -0.000056555 0.000004861 0.000151202

21 1 -0.000030499 -0.000010494 0.000092867

22 1 0.000039242 -0.000050463 -0.000133177

23 1 -0.000011720 0.000081191 -0.000080597

24 1 0.000018864 -0.000007790 0.000111860

25 1 0.000074441 0.000080149 -0.000001986

26 1 -0.000009290 -0.000076975 0.000053159

27 1 -0.000049562 -0.000002688 -0.000137997

-------------------------------------------------------------------

Cartesian Forces: Max 0.000924311 RMS 0.000254045

Leave Link 716 at Sat Aug 17 17:47:11 2019, MaxMem= 1342177280 cpu: 0.3

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.001448205 RMS 0.000182172

Search for a local minimum.

Step number 37 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .18217D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

ITU= 0 -1 -1 -1 0 -1 0 0 -1 -1 0 0 -1 0 0 -1 1 -1 1 -1

ITU= 1 1 -1 1 -1 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Use linear search instead of GDIIS.

Eigenvalues --- 0.00051 0.00149 0.00252 0.00285 0.00383

Eigenvalues --- 0.00419 0.00501 0.00762 0.01527 0.02324

Eigenvalues --- 0.02638 0.03324 0.03540 0.03640 0.04429

Eigenvalues --- 0.04746 0.04812 0.04881 0.05161 0.05440

Eigenvalues --- 0.05487 0.05536 0.05666 0.05836 0.08101

Eigenvalues --- 0.08221 0.08338 0.10867 0.11829 0.12158

Eigenvalues --- 0.13377 0.14509 0.15422 0.15913 0.15999

Eigenvalues --- 0.16015 0.16057 0.16260 0.16880 0.17411

Eigenvalues --- 0.19267 0.20014 0.21888 0.22235 0.23142

Eigenvalues --- 0.24462 0.25236 0.25605 0.26370 0.27044

Eigenvalues --- 0.27525 0.28315 0.29074 0.29210 0.29666

Eigenvalues --- 0.30617 0.31539 0.32068 0.33642 0.33859

Eigenvalues --- 0.33892 0.33910 0.33966 0.33989 0.34053

Eigenvalues --- 0.34116 0.34220 0.34320 0.34380 0.34728

Eigenvalues --- 0.34766 0.35659 0.52374 0.55329 0.86075

RFO step: Lambda=-4.29454123D-05 EMin= 5.14894052D-04

Quartic linear search produced a step of 0.18084.

Iteration 1 RMS(Cart)= 0.03106525 RMS(Int)= 0.00035203

Iteration 2 RMS(Cart)= 0.00096907 RMS(Int)= 0.00000181

Iteration 3 RMS(Cart)= 0.00000068 RMS(Int)= 0.00000180

ITry= 1 IFail=0 DXMaxC= 1.16D-01 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83732 0.00003 -0.00008 -0.00307 -0.00314 2.83418

R2 2.28684 0.00145 -0.00020 0.00237 0.00217 2.28901

R3 2.55295 0.00019 -0.00008 -0.00036 -0.00044 2.55250

R4 2.86585 0.00011 -0.00017 0.00062 0.00045 2.86631

R5 3.60029 0.00013 0.00051 0.00739 0.00791 3.60820

R6 2.05768 0.00017 -0.00003 0.00054 0.00050 2.05818

R7 1.83647 0.00025 -0.00008 0.00030 0.00023 1.83670

R8 2.06094 0.00024 -0.00006 0.00015 0.00009 2.06103

R9 2.06836 0.00013 -0.00008 -0.00005 -0.00013 2.06822

R10 2.06001 0.00007 -0.00005 -0.00007 -0.00012 2.05989

R11 3.31896 -0.00014 -0.00040 -0.00206 -0.00246 3.31650

R12 3.38442 0.00022 0.00002 0.00294 0.00296 3.38738

R13 3.25370 0.00009 -0.00008 -0.00099 -0.00107 3.25262

R14 3.47521 -0.00018 -0.00004 -0.00274 -0.00278 3.47243

R15 2.88060 0.00015 -0.00010 0.00040 0.00030 2.88090

R16 2.06367 0.00016 -0.00005 0.00051 0.00046 2.06413

R17 2.05988 0.00011 -0.00006 -0.00002 -0.00008 2.05980

R18 2.89393 0.00004 -0.00005 0.00004 -0.00001 2.89392

R19 2.07208 0.00010 -0.00006 -0.00005 -0.00011 2.07197

R20 2.07076 0.00012 -0.00004 0.00034 0.00030 2.07106

R21 2.88572 0.00012 -0.00007 0.00036 0.00029 2.88600

R22 2.07169 0.00011 -0.00005 0.00009 0.00004 2.07173

R23 2.07154 0.00008 -0.00004 0.00013 0.00009 2.07163

R24 2.06742 0.00010 -0.00005 -0.00001 -0.00006 2.06736

R25 2.06893 0.00011 -0.00006 0.00015 0.00010 2.06902

R26 2.06878 0.00010 -0.00005 0.00012 0.00007 2.06885

A1 2.17718 0.00004 -0.00007 0.00034 0.00026 2.17744

A2 1.97559 0.00006 0.00003 0.00103 0.00105 1.97664

A3 2.12996 -0.00011 0.00003 -0.00114 -0.00112 2.12885

A4 2.02400 0.00011 0.00042 0.00126 0.00168 2.02569

A5 1.83450 0.00007 -0.00073 -0.00146 -0.00220 1.83231

A6 1.87233 -0.00002 0.00014 0.00205 0.00219 1.87452

A7 1.94649 -0.00009 -0.00008 0.00047 0.00040 1.94688

A8 1.94018 -0.00001 0.00004 0.00020 0.00023 1.94041

A9 1.83353 -0.00008 0.00016 -0.00296 -0.00280 1.83073

A10 1.87337 -0.00009 -0.00018 -0.00203 -0.00221 1.87116

A11 1.91222 0.00003 0.00007 0.00075 0.00082 1.91305

A12 1.92809 -0.00007 0.00002 -0.00074 -0.00072 1.92737

A13 1.95262 -0.00006 0.00002 -0.00120 -0.00118 1.95144

A14 1.88369 0.00000 0.00001 0.00040 0.00041 1.88411

A15 1.89356 0.00002 -0.00003 0.00030 0.00026 1.89383

A16 1.89200 0.00009 -0.00009 0.00056 0.00046 1.89247

A17 1.79568 -0.00086 0.00033 0.00119 0.00152 1.79720

A18 1.97203 -0.00013 0.00018 -0.00309 -0.00291 1.96912

A19 2.14209 -0.00002 -0.00002 0.00014 0.00012 2.14221

A20 2.15411 0.00007 0.00009 0.00294 0.00303 2.15714

A21 1.79422 0.00028 -0.00006 0.00256 0.00250 1.79672

A22 1.92703 -0.00022 0.00013 -0.00113 -0.00101 1.92603

A23 1.87606 0.00016 0.00006 0.00386 0.00392 1.87998

A24 1.89410 0.00001 -0.00018 -0.00295 -0.00314 1.89096

A25 1.93919 0.00002 0.00001 0.00011 0.00012 1.93931

A26 1.93866 0.00005 0.00000 0.00028 0.00027 1.93893

A27 1.88686 -0.00001 -0.00002 -0.00010 -0.00012 1.88674

A28 1.95330 0.00006 -0.00009 -0.00010 -0.00019 1.95312

A29 1.91735 -0.00008 0.00000 -0.00142 -0.00142 1.91593

A30 1.91555 0.00005 0.00010 0.00166 0.00176 1.91731

A31 1.90643 0.00001 0.00002 0.00093 0.00095 1.90739

A32 1.90957 -0.00007 0.00002 -0.00151 -0.00149 1.90808

A33 1.85922 0.00003 -0.00005 0.00045 0.00040 1.85962

A34 1.96656 -0.00004 0.00001 -0.00043 -0.00042 1.96614

A35 1.90643 0.00001 0.00003 -0.00013 -0.00010 1.90633

A36 1.90755 0.00001 -0.00002 0.00003 0.00001 1.90756

A37 1.91260 0.00003 0.00001 0.00039 0.00040 1.91300

A38 1.91311 -0.00001 0.00002 -0.00050 -0.00047 1.91263

A39 1.85420 0.00001 -0.00006 0.00070 0.00064 1.85484

A40 1.94566 -0.00002 0.00002 -0.00041 -0.00039 1.94527

A41 1.94251 -0.00001 0.00003 -0.00063 -0.00060 1.94191

A42 1.94333 -0.00006 0.00003 -0.00047 -0.00045 1.94288

A43 1.87648 0.00002 0.00000 0.00077 0.00078 1.87726

A44 1.87671 0.00004 -0.00006 0.00069 0.00063 1.87734

A45 1.87569 0.00003 -0.00003 0.00015 0.00012 1.87582

D1 2.68430 0.00005 0.00582 0.01912 0.02493 2.70923

D2 -1.44066 0.00007 0.00543 0.01942 0.02485 -1.41581

D3 0.50453 0.00000 0.00535 0.01629 0.02163 0.52616

D4 -0.48928 -0.00004 0.00554 0.02716 0.03270 -0.45659

D5 1.66894 -0.00002 0.00515 0.02746 0.03262 1.70156

D6 -2.66905 -0.00009 0.00507 0.02433 0.02940 -2.63966

D7 -3.10463 0.00003 0.00049 -0.00347 -0.00297 -3.10760

D8 0.00595 -0.00006 0.00022 0.00436 0.00458 0.01053

D9 -3.12654 0.00001 -0.00098 -0.00202 -0.00300 -3.12954

D10 -1.05356 -0.00001 -0.00091 -0.00151 -0.00242 -1.05597

D11 1.05597 0.00001 -0.00099 -0.00213 -0.00312 1.05285

D12 1.05790 -0.00010 -0.00025 -0.00137 -0.00162 1.05628

D13 3.13089 -0.00012 -0.00018 -0.00086 -0.00104 3.12984

D14 -1.04278 -0.00010 -0.00027 -0.00148 -0.00174 -1.04452

D15 -0.98201 0.00007 -0.00043 0.00190 0.00147 -0.98053

D16 1.09098 0.00004 -0.00036 0.00241 0.00205 1.09303

D17 -3.08268 0.00006 -0.00044 0.00180 0.00135 -3.08133

D18 -3.13190 0.00018 0.00351 0.03629 0.03980 -3.09209

D19 -0.92505 0.00031 0.00348 0.03715 0.04063 -0.88442

D20 1.17859 0.00021 0.00359 0.03581 0.03940 1.21799

D21 1.83561 -0.00022 -0.00107 -0.00703 -0.00810 1.82751

D22 -1.12664 0.00026 -0.00254 -0.00728 -0.00982 -1.13646

D23 2.55667 0.00033 0.00056 0.01682 0.01737 2.57405

D24 -0.76569 -0.00016 0.00203 0.01672 0.01876 -0.74693

D25 -3.00648 -0.00008 0.00198 -0.02448 -0.02250 -3.02898

D26 -0.88869 -0.00009 0.00211 -0.02260 -0.02049 -0.90918

D27 1.14806 -0.00001 0.00202 -0.02220 -0.02019 1.12788

D28 -3.11067 0.00003 -0.00010 -0.01516 -0.01526 -3.12593

D29 -0.98979 0.00003 -0.00013 -0.01502 -0.01515 -1.00494

D30 1.04890 0.00005 -0.00013 -0.01433 -0.01446 1.03444

D31 1.09264 -0.00003 -0.00027 -0.01931 -0.01958 1.07306

D32 -3.06967 -0.00003 -0.00030 -0.01918 -0.01948 -3.08914

D33 -1.03098 -0.00002 -0.00030 -0.01849 -0.01879 -1.04976

D34 -1.00852 -0.00006 -0.00024 -0.01945 -0.01969 -1.02821

D35 1.11236 -0.00006 -0.00027 -0.01931 -0.01959 1.09277

D36 -3.13213 -0.00005 -0.00028 -0.01862 -0.01890 3.13215

D37 -3.12553 -0.00005 -0.00044 -0.01113 -0.01157 -3.13710

D38 -0.99557 -0.00004 -0.00040 -0.01101 -0.01141 -1.00698

D39 1.02626 -0.00002 -0.00047 -0.01023 -0.01070 1.01556

D40 1.03051 0.00000 -0.00040 -0.00992 -0.01032 1.02019

D41 -3.12272 0.00001 -0.00036 -0.00980 -0.01016 -3.13288

D42 -1.10089 0.00004 -0.00042 -0.00902 -0.00944 -1.11033

D43 -0.99847 0.00000 -0.00037 -0.01013 -0.01050 -1.00898

D44 1.13149 0.00001 -0.00032 -0.01002 -0.01035 1.12114

D45 -3.12987 0.00003 -0.00039 -0.00923 -0.00963 -3.13950

D46 -3.14152 0.00001 0.00017 -0.00966 -0.00949 3.13217

D47 -1.04655 0.00001 0.00021 -0.00938 -0.00917 -1.05572

D48 1.04584 0.00001 0.00021 -0.00993 -0.00972 1.03612

D49 1.01519 0.00001 0.00011 -0.00948 -0.00936 1.00583

D50 3.11016 0.00001 0.00015 -0.00920 -0.00905 3.10112

D51 -1.08063 0.00001 0.00016 -0.00975 -0.00959 -1.09022

D52 -1.01326 -0.00001 0.00017 -0.01027 -0.01010 -1.02336

D53 1.08171 -0.00001 0.00021 -0.00999 -0.00978 1.07193

D54 -3.10908 -0.00001 0.00021 -0.01054 -0.01033 -3.11941

Item Value Threshold Converged?

Maximum Force 0.001448 0.000450 NO

RMS Force 0.000182 0.000300 YES

Maximum Displacement 0.115590 0.001800 NO

RMS Displacement 0.031214 0.001200 NO

Predicted change in Energy=-2.260184D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:47:11 2019, MaxMem= 1342177280 cpu: 0.6

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.092486 -0.404598 -0.215844

2 6 0 -2.844757 0.072397 0.466063

3 8 0 -4.885377 0.312420 -0.785433

4 8 0 -4.248557 -1.745325 -0.165280

5 6 0 -2.309811 -0.815044 1.573724

6 16 0 -1.567828 0.289802 -0.936757

7 6 0 -0.114017 0.764808 -0.076011

8 16 0 1.087451 -0.560081 0.043474

9 16 0 0.011968 2.245855 0.791863

10 6 0 2.692029 0.334474 0.003106

11 6 0 3.849436 -0.655462 -0.064372

12 6 0 5.207086 0.052911 -0.077384

13 6 0 6.379192 -0.923352 -0.151132

14 1 0 -3.036985 1.081331 0.828460

15 1 0 -5.060004 -1.959072 -0.655719

16 1 0 -1.413377 -0.365338 2.002317

17 1 0 -3.050797 -0.917487 2.372650

18 1 0 -2.056862 -1.810480 1.208591

19 1 0 2.684562 0.991191 -0.869686

20 1 0 2.760077 0.957323 0.895030

21 1 0 3.804914 -1.337238 0.793172

22 1 0 3.755922 -1.276793 -0.962328

23 1 0 5.247132 0.740893 -0.930014

24 1 0 5.300984 0.672577 0.822051

25 1 0 7.338002 -0.396854 -0.168889

26 1 0 6.388788 -1.598098 0.711068

27 1 0 6.325474 -1.542398 -1.052498

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.499783 0.000000

3 O 1.211290 2.405822 0.000000

4 O 1.350727 2.381882 2.241528 0.000000

5 C 2.559091 1.516783 3.670195 2.765555 0.000000

6 S 2.715844 1.909377 3.321075 3.453003 2.841433

7 C 4.149130 2.868836 4.844977 4.837681 3.168449

8 S 5.188754 4.005106 6.092866 5.470042 3.734711

9 S 4.988679 3.604295 5.496364 5.915886 3.920596

10 C 6.828163 5.562285 7.618356 7.247458 5.367182

11 C 7.947327 6.754507 8.817805 8.171626 6.375355

12 C 9.311849 8.070186 10.120597 9.625516 7.744886

13 C 10.484720 9.298048 11.349889 10.659498 8.859213

14 H 2.100628 1.089142 2.571463 3.231936 2.163433

15 H 1.883074 3.208205 2.281885 0.971938 3.720588

16 H 3.478420 2.144886 4.503963 3.826367 1.090652

17 H 2.836983 2.158100 3.853809 2.925925 1.094457

18 H 2.854695 2.171947 4.059967 2.587526 1.090045

19 H 6.950117 5.762099 7.600776 7.486845 5.846068

20 H 7.074355 5.690455 7.854477 7.586140 5.413472

21 H 8.016038 6.805307 8.985239 8.120564 6.186422

22 H 7.931927 6.886913 8.787999 8.057697 6.590743

23 H 9.436665 8.238603 10.142594 9.845517 8.111537

24 H 9.511825 8.175576 10.318704 9.900242 7.791164

25 H 11.430587 10.213322 12.259453 11.664764 9.812843

26 H 10.589652 9.386637 11.532406 10.674398 8.776274

27 H 10.513253 9.434338 11.366392 10.613127 9.055068

6 7 8 9 10

6 S 0.000000

7 C 1.755016 0.000000

8 S 2.955277 1.792522 0.000000

9 S 3.051233 1.721213 3.096777 0.000000

10 C 4.362536 2.839954 1.837533 3.385002 0.000000

11 C 5.567884 4.210257 2.765734 4.886403 1.524506

12 C 6.833308 5.368514 4.166744 5.705597 2.532049

13 C 8.077381 6.709493 5.307764 7.174584 3.898858

14 H 2.429184 3.076036 4.507928 3.263981 5.836147

15 H 4.163137 5.676122 6.343284 6.745502 8.111005

16 H 3.015165 2.699076 3.182630 3.211718 4.619625

17 H 3.822162 4.177407 4.762132 4.678264 6.337365

18 H 3.041851 3.472313 3.578785 4.572480 5.348456

19 H 4.310367 2.917741 2.406464 3.387872 1.092291

20 H 4.746766 3.039802 2.413574 3.036949 1.090000

21 H 5.874204 4.531236 2.924145 5.217758 2.158087

22 H 5.549521 4.464316 2.940416 5.431705 2.158729

23 H 6.829876 5.428794 4.465776 5.712854 2.750353

24 H 7.100739 5.489741 4.458641 5.518133 2.755291

25 H 8.965206 7.542590 6.256287 7.847147 4.706324

26 H 8.341897 6.963426 5.443100 7.446230 4.231084

27 H 8.103985 6.909687 5.440863 7.590315 4.223609

11 12 13 14 15

11 C 0.000000

12 C 1.531397 0.000000

13 C 2.545380 1.527207 0.000000

14 H 7.157960 8.357207 9.676919 0.000000

15 H 9.023702 10.478343 11.497066 3.942010 0.000000

16 H 5.661499 6.952023 8.103879 2.471213 4.785711

17 H 7.322633 8.668159 9.761875 2.525864 3.780586

18 H 6.151330 7.608607 8.590859 3.076965 3.537880

19 H 2.171849 2.805573 4.222806 5.968913 8.290243

20 H 2.169846 2.784134 4.210628 5.798771 8.489043

21 H 1.096441 2.157885 2.773070 7.256880 9.004040

22 H 1.095957 2.158036 2.768485 7.410213 8.847601

23 H 2.157011 1.096312 2.158224 8.475536 10.658428

24 H 2.157875 1.096260 2.157917 8.347984 10.791637

25 H 3.499699 2.179785 1.093998 10.527112 12.505521

26 H 2.817478 2.178052 1.094881 9.799915 11.535738

27 H 2.809594 2.178681 1.094790 9.903414 11.400007

16 17 18 19 20

16 H 0.000000

17 H 1.767246 0.000000

18 H 1.769890 1.772111 0.000000

19 H 5.184754 6.859310 5.886400 0.000000

20 H 4.515887 6.282080 5.564347 1.766655 0.000000

21 H 5.444005 7.047817 5.895503 3.072763 2.523306

22 H 6.028393 7.588320 6.227854 2.510009 3.071280

23 H 7.361025 9.083691 8.026921 2.575471 3.092421

24 H 6.895864 8.642043 7.775145 3.131956 2.557853

25 H 9.016749 10.707830 9.599961 4.906352 4.891126

26 H 8.003800 9.608843 8.462957 4.787953 4.442023

27 H 8.402808 10.001831 8.686078 4.439453 4.770066

21 22 23 24 25

21 H 0.000000

22 H 1.757224 0.000000

23 H 3.060717 2.509145 0.000000

24 H 2.505676 3.061253 1.754223 0.000000

25 H 3.780554 3.772948 2.499103 2.505012 0.000000

26 H 2.598306 3.136157 3.076916 2.520239 1.765877

27 H 3.130785 2.584817 2.528091 3.077276 1.765856

26 27

26 H 0.000000

27 H 1.765581 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.51D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.102571 -0.465980 -0.141419

2 6 0 -2.849365 0.118883 0.438892

3 8 0 -4.899755 0.144009 -0.819383

4 8 0 -4.258585 -1.777918 0.139547

5 6 0 -2.305908 -0.566308 1.678165

6 16 0 -1.583512 0.090426 -0.990278

7 6 0 -0.122817 0.703667 -0.235039

8 16 0 1.079214 -0.583036 0.100594

9 16 0 0.010412 2.311406 0.364964

10 6 0 2.683655 0.288754 -0.105026

11 6 0 3.840235 -0.699952 -0.010686

12 6 0 5.197924 -0.006495 -0.155512

13 6 0 6.369157 -0.982830 -0.069808

14 1 0 -3.038460 1.175329 0.624357

15 1 0 -5.073940 -2.071299 -0.300666

16 1 0 -1.405996 -0.051207 2.016323

17 1 0 -3.040580 -0.529023 2.488538

18 1 0 -2.056112 -1.610022 1.487218

19 1 0 2.669457 0.786070 -1.077432

20 1 0 2.758915 1.055230 0.666305

21 1 0 3.802319 -1.224486 0.951399

22 1 0 3.739462 -1.465925 -0.788023

23 1 0 5.231405 0.525004 -1.113786

24 1 0 5.299091 0.758090 0.623565

25 1 0 7.327932 -0.468723 -0.185026

26 1 0 6.385395 -1.499727 0.895240

27 1 0 6.308152 -1.747200 -0.851205

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3033045 0.1932487 0.1807705

Leave Link 202 at Sat Aug 17 17:47:11 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.1773606365 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0549862626 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.1223743740 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2325

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.75D-11

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 110

GePol: Fraction of low-weight points (<1% of avg) = 4.73%

GePol: Cavity surface area = 309.301 Ang\*\*2

GePol: Cavity volume = 320.423 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057705238 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.1166038501 Hartrees.

Leave Link 301 at Sat Aug 17 17:47:11 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:47:12 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:47:12 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999999 0.001242 -0.000454 -0.000123 Ang= 0.15 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.63015320195

Leave Link 401 at Sat Aug 17 17:47:12 2019, MaxMem= 1342177280 cpu: 7.7

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16216875.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.55D-15 for 2310.

Iteration 1 A\*A^-1 deviation from orthogonality is 5.04D-15 for 2313 2228.

Iteration 1 A^-1\*A deviation from unit magnitude is 8.99D-15 for 2310.

Iteration 1 A^-1\*A deviation from orthogonality is 1.95D-11 for 812 763.

E= -1658.67476093278

DIIS: error= 1.27D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67476093278 IErMin= 1 ErrMin= 1.27D-03

ErrMax= 1.27D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.07D-03 BMatP= 5.07D-03

IDIUse=3 WtCom= 9.87D-01 WtEn= 1.27D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.428 Goal= None Shift= 0.000

Gap= 0.484 Goal= None Shift= 0.000

GapD= 0.428 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=1.87D-04 MaxDP=6.68D-03 OVMax= 1.01D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.87D-04 CP: 1.00D+00

E= -1658.67694538658 Delta-E= -0.002184453799 Rises=F Damp=F

DIIS: error= 1.67D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67694538658 IErMin= 2 ErrMin= 1.67D-04

ErrMax= 1.67D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.01D-04 BMatP= 5.07D-03

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.67D-03

Coeff-Com: -0.544D-01 0.105D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.543D-01 0.105D+01

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.05D-05 MaxDP=9.83D-04 DE=-2.18D-03 OVMax= 1.53D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.02D-05 CP: 1.00D+00 1.02D+00

E= -1658.67696487456 Delta-E= -0.000019487980 Rises=F Damp=F

DIIS: error= 2.30D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67696487456 IErMin= 2 ErrMin= 1.67D-04

ErrMax= 2.30D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.52D-05 BMatP= 1.01D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.30D-03

Coeff-Com: -0.336D-01 0.488D+00 0.546D+00

Coeff-En: 0.000D+00 0.912D-02 0.991D+00

Coeff: -0.336D-01 0.487D+00 0.547D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.53D-05 MaxDP=6.11D-04 DE=-1.95D-05 OVMax= 9.45D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 9.70D-06 CP: 1.00D+00 1.06D+00 6.80D-01

E= -1658.67697615525 Delta-E= -0.000011280693 Rises=F Damp=F

DIIS: error= 1.16D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67697615525 IErMin= 4 ErrMin= 1.16D-04

ErrMax= 1.16D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.18D-05 BMatP= 6.52D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.16D-03

Coeff-Com: -0.119D-01 0.161D+00 0.321D+00 0.530D+00

Coeff-En: 0.000D+00 0.000D+00 0.900D-01 0.910D+00

Coeff: -0.119D-01 0.161D+00 0.321D+00 0.531D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.91D-06 MaxDP=2.24D-04 DE=-1.13D-05 OVMax= 3.51D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.16D-06 CP: 1.00D+00 1.07D+00 7.01D-01 7.90D-01

E= -1658.67697821187 Delta-E= -0.000002056615 Rises=F Damp=F

DIIS: error= 3.17D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67697821187 IErMin= 5 ErrMin= 3.17D-05

ErrMax= 3.17D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.72D-07 BMatP= 1.18D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.341D-02 0.415D-01 0.127D+00 0.280D+00 0.555D+00

Coeff: -0.341D-02 0.415D-01 0.127D+00 0.280D+00 0.555D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.93D-06 MaxDP=7.31D-05 DE=-2.06D-06 OVMax= 2.41D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.45D-06 CP: 1.00D+00 1.07D+00 7.20D-01 8.89D-01 8.56D-01

E= -1658.67697836174 Delta-E= -0.000000149874 Rises=F Damp=F

DIIS: error= 1.40D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67697836174 IErMin= 6 ErrMin= 1.40D-05

ErrMax= 1.40D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.96D-07 BMatP= 7.72D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.428D-03-0.107D-01 0.126D-01 0.671D-01 0.360D+00 0.570D+00

Coeff: 0.428D-03-0.107D-01 0.126D-01 0.671D-01 0.360D+00 0.570D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=8.77D-07 MaxDP=3.25D-05 DE=-1.50D-07 OVMax= 7.42D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.91D-07 CP: 1.00D+00 1.07D+00 7.37D-01 9.06D-01 9.28D-01

CP: 8.54D-01

E= -1658.67697840822 Delta-E= -0.000000046479 Rises=F Damp=F

DIIS: error= 2.74D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67697840822 IErMin= 7 ErrMin= 2.74D-06

ErrMax= 2.74D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.36D-08 BMatP= 1.96D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.684D-03-0.110D-01-0.120D-01-0.962D-02 0.791D-01 0.246D+00

Coeff-Com: 0.707D+00

Coeff: 0.684D-03-0.110D-01-0.120D-01-0.962D-02 0.791D-01 0.246D+00

Coeff: 0.707D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.15D-07 MaxDP=1.32D-05 DE=-4.65D-08 OVMax= 4.95D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.74D-07 CP: 1.00D+00 1.07D+00 7.38D-01 9.29D-01 9.59D-01

CP: 9.60D-01 1.03D+00

E= -1658.67697841306 Delta-E= -0.000000004838 Rises=F Damp=F

DIIS: error= 1.23D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67697841306 IErMin= 8 ErrMin= 1.23D-06

ErrMax= 1.23D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.14D-09 BMatP= 1.36D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.214D-03-0.268D-02-0.715D-02-0.156D-01-0.248D-01 0.892D-02

Coeff-Com: 0.343D+00 0.698D+00

Coeff: 0.214D-03-0.268D-02-0.715D-02-0.156D-01-0.248D-01 0.892D-02

Coeff: 0.343D+00 0.698D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.27D-07 MaxDP=1.04D-05 DE=-4.84D-09 OVMax= 3.26D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.07D-07 CP: 1.00D+00 1.07D+00 7.39D-01 9.39D-01 9.74D-01

CP: 1.04D+00 1.22D+00 9.58D-01

E= -1658.67697841421 Delta-E= -0.000000001151 Rises=F Damp=F

DIIS: error= 6.78D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67697841421 IErMin= 9 ErrMin= 6.78D-07

ErrMax= 6.78D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.25D-10 BMatP= 3.14D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.106D-04 0.686D-03-0.182D-02-0.728D-02-0.298D-01-0.447D-01

Coeff-Com: 0.362D-01 0.371D+00 0.675D+00

Coeff: -0.106D-04 0.686D-03-0.182D-02-0.728D-02-0.298D-01-0.447D-01

Coeff: 0.362D-01 0.371D+00 0.675D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=8.75D-08 MaxDP=3.92D-06 DE=-1.15D-09 OVMax= 1.03D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 4.50D-08 CP: 1.00D+00 1.07D+00 7.40D-01 9.40D-01 9.80D-01

CP: 1.05D+00 1.29D+00 1.10D+00 7.87D-01

E= -1658.67697841443 Delta-E= -0.000000000216 Rises=F Damp=F

DIIS: error= 3.95D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67697841443 IErMin=10 ErrMin= 3.95D-07

ErrMax= 3.95D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.22D-10 BMatP= 7.25D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.427D-04 0.892D-03-0.185D-04-0.205D-02-0.146D-01-0.287D-01

Coeff-Com: -0.352D-01 0.120D+00 0.434D+00 0.525D+00

Coeff: -0.427D-04 0.892D-03-0.185D-04-0.205D-02-0.146D-01-0.287D-01

Coeff: -0.352D-01 0.120D+00 0.434D+00 0.525D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.23D-08 MaxDP=1.73D-06 DE=-2.16D-10 OVMax= 5.69D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 2.05D-08 CP: 1.00D+00 1.07D+00 7.40D-01 9.42D-01 9.79D-01

CP: 1.07D+00 1.31D+00 1.14D+00 9.29D-01 7.29D-01

E= -1658.67697841452 Delta-E= -0.000000000097 Rises=F Damp=F

DIIS: error= 1.64D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67697841452 IErMin=11 ErrMin= 1.64D-07

ErrMax= 1.64D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.39D-11 BMatP= 2.22D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.194D-04 0.335D-03 0.237D-03 0.788D-04-0.276D-02-0.717D-02

Coeff-Com: -0.251D-01 0.270D-02 0.119D+00 0.277D+00 0.635D+00

Coeff: -0.194D-04 0.335D-03 0.237D-03 0.788D-04-0.276D-02-0.717D-02

Coeff: -0.251D-01 0.270D-02 0.119D+00 0.277D+00 0.635D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.25D-08 MaxDP=7.14D-07 DE=-9.69D-11 OVMax= 1.84D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 8.45D-09 CP: 1.00D+00 1.07D+00 7.40D-01 9.42D-01 9.79D-01

CP: 1.07D+00 1.31D+00 1.16D+00 9.83D-01 8.14D-01

CP: 9.16D-01

E= -1658.67697841451 Delta-E= 0.000000000020 Rises=F Damp=F

DIIS: error= 5.43D-08 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=11 EnMin= -1658.67697841452 IErMin=12 ErrMin= 5.43D-08

ErrMax= 5.43D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.36D-12 BMatP= 2.39D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.292D-06-0.498D-04 0.119D-03 0.535D-03 0.222D-02 0.372D-02

Coeff-Com: -0.375D-02-0.284D-01-0.504D-01 0.351D-02 0.310D+00 0.762D+00

Coeff: 0.292D-06-0.498D-04 0.119D-03 0.535D-03 0.222D-02 0.372D-02

Coeff: -0.375D-02-0.284D-01-0.504D-01 0.351D-02 0.310D+00 0.762D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=7.40D-09 MaxDP=3.46D-07 DE= 1.96D-11 OVMax= 7.60D-07

Error on total polarization charges = 0.04163

SCF Done: E(UB3LYP) = -1658.67697841 A.U. after 12 cycles

NFock= 12 Conv=0.74D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655241810454D+03 PE=-6.146999264460D+03 EE= 1.730963871742D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.62

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:47:38 2019, MaxMem= 1342177280 cpu: 303.7

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 340

Leave Link 701 at Sat Aug 17 17:47:39 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:47:39 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:47:43 2019, MaxMem= 1342177280 cpu: 38.1

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.40188394D+00-2.94413471D+00 6.24380142D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000794302 0.000091179 0.001096040

2 6 0.000701530 0.000152132 0.000274680

3 8 0.000182603 0.000203521 -0.000537192

4 8 0.000196980 -0.000213476 -0.000442433

5 6 0.000053637 -0.000006145 -0.000296090

6 16 -0.000129300 0.000039177 0.000006822

7 6 0.000001736 -0.000348032 -0.000324502

8 16 -0.000120042 0.000012332 -0.000001332

9 16 0.000157392 0.000065157 0.000224277

10 6 -0.000178335 0.000111330 0.000093501

11 6 0.000079319 0.000009981 -0.000047925

12 6 -0.000046405 0.000007457 0.000083568

13 6 -0.000077752 -0.000039948 0.000004994

14 1 -0.000180129 -0.000041852 0.000024990

15 1 -0.000116259 -0.000126255 -0.000109676

16 1 0.000084886 0.000031713 -0.000011817

17 1 -0.000066261 0.000035038 0.000048557

18 1 -0.000033161 -0.000149478 -0.000016376

19 1 -0.000042505 0.000028122 -0.000048804

20 1 0.000160520 0.000069719 0.000120148

21 1 0.000023758 -0.000049911 0.000046290

22 1 -0.000055240 0.000012758 -0.000068265

23 1 -0.000017077 0.000075106 -0.000017455

24 1 0.000048842 0.000035239 0.000061215

25 1 0.000115531 0.000006168 0.000027006

26 1 0.000028670 -0.000075035 -0.000022583

27 1 0.000021362 0.000064002 -0.000167636

-------------------------------------------------------------------

Cartesian Forces: Max 0.001096040 RMS 0.000217427

Leave Link 716 at Sat Aug 17 17:47:43 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000467507 RMS 0.000137380

Search for a local minimum.

Step number 38 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .13738D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38

DE= 1.82D-05 DEPred=-2.26D-05 R=-8.06D-01

Trust test=-8.06D-01 RLast= 1.29D-01 DXMaxT set to 5.00D-02

ITU= -1 0 -1 -1 -1 0 -1 0 0 -1 -1 0 0 -1 0 0 -1 1 -1 1

ITU= -1 1 1 -1 1 -1 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Eigenvalues --- 0.00068 0.00229 0.00287 0.00296 0.00309

Eigenvalues --- 0.00416 0.00463 0.01117 0.01502 0.02295

Eigenvalues --- 0.02530 0.03521 0.03577 0.04294 0.04623

Eigenvalues --- 0.04786 0.04835 0.04957 0.05258 0.05451

Eigenvalues --- 0.05491 0.05563 0.05672 0.05826 0.08218

Eigenvalues --- 0.08308 0.08397 0.10994 0.12016 0.12186

Eigenvalues --- 0.13213 0.14428 0.15602 0.15946 0.16001

Eigenvalues --- 0.16045 0.16227 0.16261 0.17009 0.17722

Eigenvalues --- 0.19601 0.20170 0.21875 0.22184 0.23278

Eigenvalues --- 0.24155 0.25145 0.25336 0.26453 0.27068

Eigenvalues --- 0.27814 0.28246 0.29092 0.29404 0.29623

Eigenvalues --- 0.30312 0.31623 0.32613 0.33762 0.33877

Eigenvalues --- 0.33916 0.33928 0.33950 0.34037 0.34071

Eigenvalues --- 0.34130 0.34236 0.34340 0.34598 0.34685

Eigenvalues --- 0.34877 0.35401 0.52463 0.56107 0.87903

En-DIIS/RFO-DIIS IScMMF= 0 using points: 38 37

RFO step: Lambda=-7.00861702D-06.

NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=F DC= -1.82D-05 SmlDif= 1.00D-05

RMS Error= 0.5808717049D-03 NUsed= 2 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.70301 0.29699

Iteration 1 RMS(Cart)= 0.03388046 RMS(Int)= 0.00040810

Iteration 2 RMS(Cart)= 0.00058450 RMS(Int)= 0.00000948

Iteration 3 RMS(Cart)= 0.00000014 RMS(Int)= 0.00000948

ITry= 1 IFail=0 DXMaxC= 1.07D-01 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83418 0.00046 0.00093 0.00043 0.00137 2.83555

R2 2.28901 0.00025 -0.00064 0.00038 -0.00026 2.28874

R3 2.55250 0.00036 0.00013 0.00079 0.00092 2.55343

R4 2.86631 -0.00020 -0.00013 -0.00162 -0.00176 2.86455

R5 3.60820 0.00003 -0.00235 0.00998 0.00763 3.61583

R6 2.05818 0.00000 -0.00015 0.00027 0.00012 2.05830

R7 1.83670 0.00016 -0.00007 0.00017 0.00010 1.83680

R8 2.06103 0.00010 -0.00003 0.00012 0.00010 2.06113

R9 2.06822 0.00008 0.00004 0.00004 0.00008 2.06830

R10 2.05989 0.00009 0.00004 0.00018 0.00022 2.06010

R11 3.31650 0.00003 0.00073 -0.00443 -0.00370 3.31280

R12 3.38738 -0.00017 -0.00088 0.00265 0.00178 3.38915

R13 3.25262 0.00016 0.00032 -0.00071 -0.00039 3.25223

R14 3.47243 0.00014 0.00083 -0.00175 -0.00092 3.47151

R15 2.88090 0.00010 -0.00009 0.00031 0.00022 2.88112

R16 2.06413 0.00007 -0.00014 0.00023 0.00010 2.06423

R17 2.05980 0.00013 0.00002 0.00016 0.00019 2.05999

R18 2.89392 0.00008 0.00000 0.00005 0.00005 2.89397

R19 2.07197 0.00008 0.00003 -0.00008 -0.00004 2.07193

R20 2.07106 0.00004 -0.00009 0.00017 0.00009 2.07114

R21 2.88600 0.00012 -0.00008 0.00056 0.00048 2.88648

R22 2.07173 0.00006 -0.00001 -0.00009 -0.00010 2.07163

R23 2.07163 0.00007 -0.00003 0.00021 0.00019 2.07182

R24 2.06736 0.00010 0.00002 0.00015 0.00017 2.06752

R25 2.06902 0.00005 -0.00003 -0.00011 -0.00013 2.06889

R26 2.06885 0.00008 -0.00002 0.00024 0.00022 2.06907

A1 2.17744 -0.00021 -0.00008 -0.00024 -0.00037 2.17707

A2 1.97664 0.00016 -0.00031 0.00074 0.00038 1.97702

A3 2.12885 0.00003 0.00033 -0.00087 -0.00060 2.12825

A4 2.02569 0.00022 -0.00050 0.00477 0.00426 2.02995

A5 1.83231 -0.00015 0.00065 -0.00689 -0.00623 1.82608

A6 1.87452 -0.00011 -0.00065 0.00243 0.00177 1.87629

A7 1.94688 -0.00004 -0.00012 -0.00115 -0.00126 1.94562

A8 1.94041 -0.00002 -0.00007 0.00073 0.00066 1.94107

A9 1.83073 0.00009 0.00083 -0.00064 0.00019 1.83093

A10 1.87116 0.00023 0.00066 0.00060 0.00125 1.87241

A11 1.91305 -0.00010 -0.00024 0.00054 0.00029 1.91334

A12 1.92737 -0.00011 0.00021 -0.00072 -0.00051 1.92686

A13 1.95144 0.00012 0.00035 0.00030 0.00065 1.95209

A14 1.88411 0.00005 -0.00012 -0.00027 -0.00039 1.88372

A15 1.89383 0.00003 -0.00008 0.00005 -0.00003 1.89380

A16 1.89247 0.00001 -0.00014 0.00009 -0.00005 1.89241

A17 1.79720 -0.00014 -0.00045 0.00430 0.00385 1.80105

A18 1.96912 0.00041 0.00086 -0.00090 -0.00007 1.96906

A19 2.14221 0.00004 -0.00003 0.00180 0.00174 2.14395

A20 2.15714 -0.00047 -0.00090 0.00134 0.00041 2.15755

A21 1.79672 -0.00040 -0.00074 0.00109 0.00035 1.79707

A22 1.92603 0.00003 0.00030 -0.00010 0.00020 1.92623

A23 1.87998 -0.00004 -0.00116 0.00247 0.00130 1.88128

A24 1.89096 0.00010 0.00093 -0.00105 -0.00012 1.89084

A25 1.93931 0.00000 -0.00004 -0.00013 -0.00017 1.93915

A26 1.93893 -0.00010 -0.00008 -0.00090 -0.00098 1.93795

A27 1.88674 0.00003 0.00004 -0.00022 -0.00019 1.88656

A28 1.95312 0.00006 0.00006 0.00014 0.00019 1.95331

A29 1.91593 0.00004 0.00042 -0.00046 -0.00004 1.91590

A30 1.91731 -0.00009 -0.00052 0.00094 0.00042 1.91773

A31 1.90739 -0.00008 -0.00028 -0.00007 -0.00036 1.90703

A32 1.90808 0.00006 0.00044 -0.00050 -0.00005 1.90803

A33 1.85962 0.00002 -0.00012 -0.00006 -0.00018 1.85944

A34 1.96614 -0.00003 0.00012 -0.00037 -0.00025 1.96589

A35 1.90633 0.00003 0.00003 0.00027 0.00030 1.90663

A36 1.90756 0.00001 0.00000 0.00018 0.00017 1.90773

A37 1.91300 -0.00001 -0.00012 -0.00025 -0.00037 1.91263

A38 1.91263 0.00002 0.00014 0.00055 0.00069 1.91332

A39 1.85484 -0.00001 -0.00019 -0.00037 -0.00056 1.85428

A40 1.94527 0.00006 0.00012 0.00041 0.00052 1.94579

A41 1.94191 0.00006 0.00018 0.00010 0.00028 1.94219

A42 1.94288 -0.00006 0.00013 -0.00066 -0.00053 1.94236

A43 1.87726 -0.00006 -0.00023 0.00038 0.00015 1.87741

A44 1.87734 -0.00003 -0.00019 -0.00065 -0.00084 1.87650

A45 1.87582 0.00002 -0.00004 0.00043 0.00039 1.87621

D1 2.70923 0.00029 -0.00741 0.05351 0.04611 2.75535

D2 -1.41581 0.00026 -0.00738 0.04984 0.04246 -1.37335

D3 0.52616 0.00024 -0.00643 0.04708 0.04065 0.56682

D4 -0.45659 -0.00027 -0.00971 0.03635 0.02665 -0.42994

D5 1.70156 -0.00030 -0.00969 0.03268 0.02300 1.72455

D6 -2.63966 -0.00031 -0.00873 0.02993 0.02119 -2.61847

D7 -3.10760 0.00028 0.00088 0.01267 0.01355 -3.09405

D8 0.01053 -0.00026 -0.00136 -0.00394 -0.00530 0.00523

D9 -3.12954 -0.00003 0.00089 -0.02218 -0.02129 3.13235

D10 -1.05597 -0.00009 0.00072 -0.02261 -0.02189 -1.07787

D11 1.05285 -0.00007 0.00093 -0.02280 -0.02187 1.03097

D12 1.05628 0.00005 0.00048 -0.01559 -0.01511 1.04117

D13 3.12984 -0.00002 0.00031 -0.01602 -0.01571 3.11414

D14 -1.04452 0.00000 0.00052 -0.01621 -0.01569 -1.06021

D15 -0.98053 -0.00002 -0.00044 -0.01453 -0.01497 -0.99550

D16 1.09303 -0.00008 -0.00061 -0.01496 -0.01557 1.07746

D17 -3.08133 -0.00007 -0.00040 -0.01515 -0.01555 -3.09688

D18 -3.09209 -0.00006 -0.01182 0.04501 0.03319 -3.05891

D19 -0.88442 0.00009 -0.01207 0.04548 0.03342 -0.85099

D20 1.21799 0.00009 -0.01170 0.04535 0.03365 1.25164

D21 1.82751 -0.00002 0.00241 -0.00901 -0.00660 1.82092

D22 -1.13646 0.00015 0.00292 -0.02251 -0.01960 -1.15606

D23 2.57405 0.00026 -0.00516 0.02103 0.01588 2.58992

D24 -0.74693 0.00015 -0.00557 0.03473 0.02916 -0.71777

D25 -3.02898 0.00002 0.00668 0.00218 0.00886 -3.02012

D26 -0.90918 0.00000 0.00609 0.00352 0.00960 -0.89958

D27 1.12788 0.00007 0.00599 0.00402 0.01002 1.13790

D28 -3.12593 0.00001 0.00453 -0.01042 -0.00589 -3.13181

D29 -1.00494 -0.00002 0.00450 -0.01073 -0.00623 -1.01118

D30 1.03444 -0.00003 0.00430 -0.01053 -0.00624 1.02820

D31 1.07306 0.00005 0.00582 -0.01336 -0.00754 1.06552

D32 -3.08914 0.00002 0.00578 -0.01367 -0.00789 -3.09703

D33 -1.04976 0.00000 0.00558 -0.01347 -0.00789 -1.05765

D34 -1.02821 0.00009 0.00585 -0.01239 -0.00654 -1.03475

D35 1.09277 0.00005 0.00582 -0.01270 -0.00689 1.08589

D36 3.13215 0.00004 0.00561 -0.01250 -0.00689 3.12527

D37 -3.13710 0.00006 0.00344 0.00561 0.00905 -3.12805

D38 -1.00698 0.00004 0.00339 0.00524 0.00863 -0.99835

D39 1.01556 0.00005 0.00318 0.00504 0.00822 1.02378

D40 1.02019 0.00003 0.00306 0.00615 0.00921 1.02940

D41 -3.13288 0.00002 0.00302 0.00577 0.00879 -3.12409

D42 -1.11033 0.00002 0.00280 0.00558 0.00838 -1.10196

D43 -1.00898 0.00003 0.00312 0.00654 0.00966 -0.99931

D44 1.12114 0.00001 0.00307 0.00617 0.00924 1.13038

D45 -3.13950 0.00001 0.00286 0.00597 0.00883 -3.13067

D46 3.13217 0.00002 0.00282 0.00681 0.00963 -3.14138

D47 -1.05572 0.00002 0.00272 0.00765 0.01037 -1.04535

D48 1.03612 0.00005 0.00289 0.00781 0.01070 1.04682

D49 1.00583 0.00001 0.00278 0.00690 0.00968 1.01551

D50 3.10112 0.00002 0.00269 0.00773 0.01042 3.11153

D51 -1.09022 0.00004 0.00285 0.00790 0.01075 -1.07948

D52 -1.02336 0.00003 0.00300 0.00718 0.01017 -1.01318

D53 1.07193 0.00003 0.00290 0.00801 0.01091 1.08284

D54 -3.11941 0.00005 0.00307 0.00818 0.01124 -3.10817

Item Value Threshold Converged?

Maximum Force 0.000468 0.000450 NO

RMS Force 0.000137 0.000300 YES

Maximum Displacement 0.106660 0.001800 NO

RMS Displacement 0.033913 0.001200 NO

Predicted change in Energy=-2.113795D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:47:43 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.083473 -0.429445 -0.224802

2 6 0 -2.853441 0.081947 0.465866

3 8 0 -4.865335 0.259610 -0.841875

4 8 0 -4.223128 -1.770920 -0.142790

5 6 0 -2.300667 -0.782923 1.581326

6 16 0 -1.574123 0.317650 -0.937326

7 6 0 -0.117692 0.778958 -0.077553

8 16 0 1.078308 -0.553202 0.029402

9 16 0 0.026587 2.260633 0.785978

10 6 0 2.686382 0.334914 0.020157

11 6 0 3.840249 -0.657799 -0.066901

12 6 0 5.200718 0.045316 -0.063183

13 6 0 6.368626 -0.933428 -0.168951

14 1 0 -3.070801 1.089167 0.818901

15 1 0 -5.016105 -2.010300 -0.651374

16 1 0 -1.407431 -0.316214 1.998391

17 1 0 -3.035518 -0.883184 2.386229

18 1 0 -2.037447 -1.780367 1.228808

19 1 0 2.687179 1.014887 -0.834740

20 1 0 2.752835 0.933442 0.928819

21 1 0 3.792208 -1.357211 0.776098

22 1 0 3.745782 -1.260051 -0.977720

23 1 0 5.241580 0.757536 -0.895561

24 1 0 5.299486 0.638801 0.853343

25 1 0 7.330321 -0.411750 -0.164408

26 1 0 6.371962 -1.639900 0.667406

27 1 0 6.315098 -1.517805 -1.093320

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.500507 0.000000

3 O 1.211150 2.406132 0.000000

4 O 1.351216 2.383196 2.241473 0.000000

5 C 2.562311 1.515853 3.679171 2.764882 0.000000

6 S 2.713426 1.913415 3.293108 3.465637 2.843015

7 C 4.148414 2.874970 4.836737 4.833295 3.155429

8 S 5.169518 4.006565 6.061904 5.442216 3.725414

9 S 5.015056 3.625425 5.530362 5.930945 3.913045

10 C 6.817271 5.563478 7.601132 7.225124 5.343919

11 C 7.928584 6.755483 8.788027 8.140199 6.359493

12 C 9.297727 8.071599 10.098402 9.597601 7.724065

13 C 10.464391 9.299489 11.317157 10.624845 8.845494

14 H 2.102618 1.089207 2.581995 3.229986 2.163127

15 H 1.884375 3.209803 2.282873 0.971994 3.723574

16 H 3.480892 2.144320 4.511739 3.824785 1.090703

17 H 2.849837 2.156948 3.882636 2.931627 1.094499

18 H 2.850297 2.171667 4.055389 2.580421 1.090159

19 H 6.949809 5.767185 7.590189 7.482771 5.826500

20 H 7.065650 5.689438 7.850219 7.558174 5.376761

21 H 7.993054 6.806767 8.954608 8.078436 6.172628

22 H 7.909110 6.887281 8.745237 8.028800 6.583002

23 H 9.424195 8.236459 10.119315 9.825500 8.086623

24 H 9.504918 8.181103 10.312185 9.873157 7.766183

25 H 11.413968 10.215185 12.232895 11.633143 9.794963

26 H 10.563019 9.386876 11.496214 10.626831 8.762657

27 H 10.491384 9.436756 11.323626 10.584034 9.051253

6 7 8 9 10

6 S 0.000000

7 C 1.753056 0.000000

8 S 2.954376 1.793462 0.000000

9 S 3.050776 1.721006 3.097771 0.000000

10 C 4.366804 2.840696 1.837046 3.371851 0.000000

11 C 5.569970 4.210663 2.765598 4.877362 1.524621

12 C 6.836430 5.368792 4.166661 5.692129 2.532331

13 C 8.077305 6.709168 5.307672 7.164870 3.899150

14 H 2.433027 3.101727 4.531643 3.311681 5.861062

15 H 4.165136 5.666011 6.303051 6.762809 8.079560

16 H 3.007991 2.678129 3.179934 3.188494 4.593113

17 H 3.824094 4.164931 4.752587 4.671282 6.310483

18 H 3.050980 3.455746 3.557026 4.559168 5.315055

19 H 4.319185 2.914841 2.407096 3.355199 1.092343

20 H 4.752291 3.045748 2.413111 3.035501 1.090100

21 H 5.876946 4.536437 2.927327 5.221953 2.158144

22 H 5.549068 4.460301 2.937575 5.416479 2.159166

23 H 6.830011 5.421383 4.461662 5.681815 2.747032

24 H 7.110284 5.498367 4.462970 5.517095 2.759504

25 H 8.967640 7.543092 6.256616 7.835139 4.707201

26 H 8.339511 6.965735 5.441576 7.449295 4.231114

27 H 8.101422 6.905627 5.441961 7.573223 4.223740

11 12 13 14 15

11 C 0.000000

12 C 1.531425 0.000000

13 C 2.545403 1.527460 0.000000

14 H 7.183255 8.383659 9.704098 0.000000

15 H 8.978077 10.438151 11.445719 3.943680 0.000000

16 H 5.649801 6.931698 8.096011 2.476508 4.786827

17 H 7.303753 8.642761 9.745224 2.519510 3.797387

18 H 6.122608 7.575843 8.563474 3.077348 3.529923

19 H 2.171872 2.802365 4.218087 5.991192 8.278041

20 H 2.169326 2.786570 4.214765 5.826755 8.456894

21 H 1.096418 2.157632 2.776803 7.286117 8.947099

22 H 1.096003 2.158054 2.764073 7.430510 8.800002

23 H 2.157216 1.096257 2.158137 8.493823 10.627353

24 H 2.158100 1.096358 2.158715 8.382466 10.756084

25 H 3.500094 2.180451 1.094087 10.554762 12.459002

26 H 2.813059 2.178423 1.094809 9.830389 11.470155

27 H 2.813898 2.178616 1.094906 9.927134 11.350508

16 17 18 19 20

16 H 0.000000

17 H 1.767071 0.000000

18 H 1.770006 1.772204 0.000000

19 H 5.154056 6.835684 5.864620 0.000000

20 H 4.473638 6.239327 5.513761 1.766660 0.000000

21 H 5.441868 7.031008 5.862499 3.072904 2.520062

22 H 6.025252 7.579195 6.211701 2.513250 3.071196

23 H 7.330569 9.053864 7.996132 2.568052 3.090818

24 H 6.870657 8.610370 7.734594 3.132924 2.564750

25 H 9.001952 10.685440 9.569182 4.903408 4.894698

26 H 8.002664 9.593105 8.429298 4.783510 4.448428

27 H 8.404758 9.997201 8.673305 4.432063 4.773612

21 22 23 24 25

21 H 0.000000

22 H 1.757121 0.000000

23 H 3.060601 2.512930 0.000000

24 H 2.502382 3.061442 1.753886 0.000000

25 H 3.781097 3.772269 2.502930 2.502752 0.000000

26 H 2.597471 3.122106 3.077066 2.525323 1.765989

27 H 3.144119 2.584799 2.523633 3.077647 1.765478

26 27

26 H 0.000000

27 H 1.765870 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 4.05D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.095798 -0.487936 -0.137150

2 6 0 -2.858865 0.132009 0.443526

3 8 0 -4.882145 0.085725 -0.857883

4 8 0 -4.236696 -1.794309 0.178007

5 6 0 -2.297386 -0.527471 1.687567

6 16 0 -1.591839 0.116364 -0.990196

7 6 0 -0.127073 0.715699 -0.236232

8 16 0 1.067866 -0.581192 0.090414

9 16 0 0.027139 2.324475 0.355310

10 6 0 2.677105 0.286943 -0.086872

11 6 0 3.828675 -0.709267 -0.009926

12 6 0 5.190162 -0.020315 -0.140163

13 6 0 6.355624 -1.006063 -0.084191

14 1 0 -3.071559 1.185912 0.617944

15 1 0 -5.034557 -2.116053 -0.274399

16 1 0 -1.399755 0.001931 2.009473

17 1 0 -3.025134 -0.484082 2.503917

18 1 0 -2.038815 -1.571795 1.511566

19 1 0 2.671239 0.807962 -1.046933

20 1 0 2.752593 1.034099 0.703304

21 1 0 3.787164 -1.251355 0.942203

22 1 0 3.725150 -1.460380 -0.801338

23 1 0 5.224607 0.536254 -1.083998

24 1 0 5.298026 0.723144 0.658356

25 1 0 7.318092 -0.494440 -0.178653

26 1 0 6.365418 -1.556414 0.862184

27 1 0 6.292941 -1.742053 -0.892404

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2866130 0.1940315 0.1813064

Leave Link 202 at Sat Aug 17 17:47:43 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.5059866316 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0550073539 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.4509792777 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2319

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.38D-09

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 92

GePol: Fraction of low-weight points (<1% of avg) = 3.97%

GePol: Cavity surface area = 309.078 Ang\*\*2

GePol: Cavity volume = 320.342 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057830033 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.4451962745 Hartrees.

Leave Link 301 at Sat Aug 17 17:47:43 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:47:43 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:47:43 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999996 0.002948 -0.000165 0.000256 Ang= 0.34 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.63035185271

Leave Link 401 at Sat Aug 17 17:47:44 2019, MaxMem= 1342177280 cpu: 7.6

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16133283.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.55D-15 for 2285.

Iteration 1 A\*A^-1 deviation from orthogonality is 1.87D-15 for 708 445.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.00D-15 for 2285.

Iteration 1 A^-1\*A deviation from orthogonality is 1.87D-12 for 750 715.

E= -1658.67376681522

DIIS: error= 1.70D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67376681522 IErMin= 1 ErrMin= 1.70D-03

ErrMax= 1.70D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.57D-03 BMatP= 7.57D-03

IDIUse=3 WtCom= 9.83D-01 WtEn= 1.70D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.428 Goal= None Shift= 0.000

Gap= 0.484 Goal= None Shift= 0.000

GapD= 0.428 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=1.84D-04 MaxDP=5.17D-03 OVMax= 1.22D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.84D-04 CP: 1.00D+00

E= -1658.67693186496 Delta-E= -0.003165049746 Rises=F Damp=F

DIIS: error= 2.89D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67693186496 IErMin= 2 ErrMin= 2.89D-04

ErrMax= 2.89D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.24D-04 BMatP= 7.57D-03

IDIUse=3 WtCom= 9.97D-01 WtEn= 2.89D-03

Coeff-Com: -0.645D-01 0.106D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.643D-01 0.106D+01

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.12D-05 MaxDP=1.28D-03 DE=-3.17D-03 OVMax= 2.41D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.86D-05 CP: 1.00D+00 1.07D+00

E= -1658.67696017567 Delta-E= -0.000028310703 Rises=F Damp=F

DIIS: error= 3.62D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67696017567 IErMin= 2 ErrMin= 2.89D-04

ErrMax= 3.62D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.54D-05 BMatP= 1.24D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.62D-03

Coeff-Com: -0.360D-01 0.497D+00 0.539D+00

Coeff-En: 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.359D-01 0.495D+00 0.541D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.54D-05 MaxDP=6.45D-04 DE=-2.83D-05 OVMax= 1.57D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.07D-05 CP: 1.00D+00 1.09D+00 6.36D-01

E= -1658.67697061711 Delta-E= -0.000010441443 Rises=F Damp=F

DIIS: error= 2.33D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67697061711 IErMin= 4 ErrMin= 2.33D-04

ErrMax= 2.33D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.34D-05 BMatP= 7.54D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.33D-03

Coeff-Com: -0.127D-01 0.163D+00 0.358D+00 0.492D+00

Coeff-En: 0.000D+00 0.000D+00 0.239D+00 0.761D+00

Coeff: -0.127D-01 0.162D+00 0.358D+00 0.492D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.47D-06 MaxDP=2.45D-04 DE=-1.04D-05 OVMax= 7.21D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.79D-06 CP: 1.00D+00 1.09D+00 7.16D-01 6.72D-01

E= -1658.67697463151 Delta-E= -0.000004014399 Rises=F Damp=F

DIIS: error= 3.59D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67697463151 IErMin= 5 ErrMin= 3.59D-05

ErrMax= 3.59D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.42D-06 BMatP= 2.34D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.387D-02 0.450D-01 0.156D+00 0.278D+00 0.525D+00

Coeff: -0.387D-02 0.450D-01 0.156D+00 0.278D+00 0.525D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.72D-06 MaxDP=9.95D-05 DE=-4.01D-06 OVMax= 1.32D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.26D-06 CP: 1.00D+00 1.09D+00 7.38D-01 7.36D-01 8.51D-01

E= -1658.67697489269 Delta-E= -0.000000261186 Rises=F Damp=F

DIIS: error= 1.21D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67697489269 IErMin= 6 ErrMin= 1.21D-05

ErrMax= 1.21D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.55D-07 BMatP= 1.42D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.320D-03-0.872D-02 0.172D-01 0.609D-01 0.277D+00 0.654D+00

Coeff: 0.320D-03-0.872D-02 0.172D-01 0.609D-01 0.277D+00 0.654D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=8.74D-07 MaxDP=6.18D-05 DE=-2.61D-07 OVMax= 1.09D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.90D-07 CP: 1.00D+00 1.09D+00 7.57D-01 7.54D-01 9.06D-01

CP: 9.31D-01

E= -1658.67697492494 Delta-E= -0.000000032245 Rises=F Damp=F

DIIS: error= 2.94D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67697492494 IErMin= 7 ErrMin= 2.94D-06

ErrMax= 2.94D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.49D-08 BMatP= 1.55D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.527D-03-0.864D-02-0.670D-02 0.248D-02 0.750D-01 0.302D+00

Coeff-Com: 0.636D+00

Coeff: 0.527D-03-0.864D-02-0.670D-02 0.248D-02 0.750D-01 0.302D+00

Coeff: 0.636D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.76D-07 MaxDP=1.44D-05 DE=-3.22D-08 OVMax= 5.48D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.58D-07 CP: 1.00D+00 1.09D+00 7.58D-01 7.64D-01 9.51D-01

CP: 1.01D+00 1.01D+00

E= -1658.67697492935 Delta-E= -0.000000004412 Rises=F Damp=F

DIIS: error= 9.33D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67697492935 IErMin= 8 ErrMin= 9.33D-07

ErrMax= 9.33D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.92D-09 BMatP= 1.49D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.125D-03-0.148D-02-0.475D-02-0.789D-02-0.165D-01 0.512D-02

Coeff-Com: 0.242D+00 0.784D+00

Coeff: 0.125D-03-0.148D-02-0.475D-02-0.789D-02-0.165D-01 0.512D-02

Coeff: 0.242D+00 0.784D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.17D-07 MaxDP=1.04D-05 DE=-4.41D-09 OVMax= 3.36D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 9.56D-08 CP: 1.00D+00 1.09D+00 7.60D-01 7.68D-01 9.69D-01

CP: 1.09D+00 1.20D+00 1.01D+00

E= -1658.67697493032 Delta-E= -0.000000000975 Rises=F Damp=F

DIIS: error= 5.12D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67697493032 IErMin= 9 ErrMin= 5.12D-07

ErrMax= 5.12D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.34D-10 BMatP= 1.92D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.449D-04 0.109D-02-0.113D-02-0.476D-02-0.251D-01-0.611D-01

Coeff-Com: -0.887D-02 0.414D+00 0.686D+00

Coeff: -0.449D-04 0.109D-02-0.113D-02-0.476D-02-0.251D-01-0.611D-01

Coeff: -0.887D-02 0.414D+00 0.686D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.14D-07 MaxDP=4.78D-06 DE=-9.75D-10 OVMax= 1.71D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 4.50D-08 CP: 1.00D+00 1.09D+00 7.62D-01 7.70D-01 9.78D-01

CP: 1.11D+00 1.29D+00 1.25D+00 8.91D-01

E= -1658.67697493056 Delta-E= -0.000000000241 Rises=F Damp=F

DIIS: error= 3.17D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67697493056 IErMin=10 ErrMin= 3.17D-07

ErrMax= 3.17D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.68D-10 BMatP= 6.34D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.524D-04 0.979D-03 0.241D-03-0.139D-02-0.121D-01-0.392D-01

Coeff-Com: -0.606D-01 0.901D-01 0.407D+00 0.615D+00

Coeff: -0.524D-04 0.979D-03 0.241D-03-0.139D-02-0.121D-01-0.392D-01

Coeff: -0.606D-01 0.901D-01 0.407D+00 0.615D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.87D-08 MaxDP=2.39D-06 DE=-2.41D-10 OVMax= 6.00D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 2.17D-08 CP: 1.00D+00 1.09D+00 7.62D-01 7.70D-01 9.79D-01

CP: 1.12D+00 1.32D+00 1.29D+00 1.01D+00 7.97D-01

E= -1658.67697493063 Delta-E= -0.000000000068 Rises=F Damp=F

DIIS: error= 1.26D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67697493063 IErMin=11 ErrMin= 1.26D-07

ErrMax= 1.26D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.54D-11 BMatP= 1.68D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.182D-04 0.283D-03 0.346D-03 0.221D-03-0.106D-02-0.745D-02

Coeff-Com: -0.282D-01-0.303D-01 0.750D-01 0.361D+00 0.630D+00

Coeff: -0.182D-04 0.283D-03 0.346D-03 0.221D-03-0.106D-02-0.745D-02

Coeff: -0.282D-01-0.303D-01 0.750D-01 0.361D+00 0.630D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.10D-08 MaxDP=8.81D-07 DE=-6.82D-11 OVMax= 3.12D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.07D-08 CP: 1.00D+00 1.09D+00 7.62D-01 7.70D-01 9.80D-01

CP: 1.13D+00 1.33D+00 1.32D+00 1.07D+00 9.82D-01

CP: 8.00D-01

E= -1658.67697493063 Delta-E= 0.000000000005 Rises=F Damp=F

DIIS: error= 6.95D-08 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=11 EnMin= -1658.67697493063 IErMin=12 ErrMin= 6.95D-08

ErrMax= 6.95D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.04D-12 BMatP= 3.54D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.167D-06-0.325D-04 0.128D-03 0.350D-03 0.162D-02 0.322D-02

Coeff-Com: -0.475D-02-0.349D-01-0.423D-01 0.801D-01 0.330D+00 0.667D+00

Coeff: -0.167D-06-0.325D-04 0.128D-03 0.350D-03 0.162D-02 0.322D-02

Coeff: -0.475D-02-0.349D-01-0.423D-01 0.801D-01 0.330D+00 0.667D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.77D-09 MaxDP=3.68D-07 DE= 5.00D-12 OVMax= 6.86D-07

Error on total polarization charges = 0.04163

SCF Done: E(UB3LYP) = -1658.67697493 A.U. after 12 cycles

NFock= 12 Conv=0.68D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655238200894D+03 PE=-6.147660025210D+03 EE= 1.731299653111D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.63

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:48:10 2019, MaxMem= 1342177280 cpu: 303.1

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 337

Leave Link 701 at Sat Aug 17 17:48:11 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:48:11 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:48:14 2019, MaxMem= 1342177280 cpu: 38.5

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.41242323D+00-2.94513999D+00 6.72677027D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000944448 -0.000598378 -0.000267270

2 6 0.000025165 0.000260895 0.000252235

3 8 -0.000499752 0.000674416 -0.000073085

4 8 0.000033743 -0.000082720 0.000193865

5 6 -0.000059815 -0.000179345 -0.000047295

6 16 -0.000215038 -0.000102863 -0.000065081

7 6 0.000171528 -0.000339802 -0.000570305

8 16 -0.000231515 0.000237400 -0.000019110

9 16 0.000100694 0.000061770 0.000437668

10 6 0.000076000 0.000053837 0.000234605

11 6 0.000068366 -0.000067420 -0.000093885

12 6 0.000100835 0.000001504 0.000137336

13 6 -0.000113355 0.000166092 -0.000121979

14 1 -0.000197935 -0.000009479 0.000045955

15 1 -0.000067052 0.000048550 -0.000027558

16 1 -0.000004811 -0.000034857 0.000041398

17 1 -0.000065575 -0.000029244 0.000014526

18 1 -0.000042815 -0.000044111 -0.000006410

19 1 -0.000140687 -0.000081752 -0.000045260

20 1 0.000115608 0.000116608 0.000002787

21 1 0.000001787 -0.000074039 0.000033587

22 1 -0.000040162 0.000072307 -0.000075613

23 1 -0.000013716 0.000051930 -0.000096357

24 1 0.000003371 -0.000030955 0.000026773

25 1 0.000022030 0.000048969 0.000028106

26 1 0.000038426 -0.000070169 0.000056340

27 1 -0.000009771 -0.000049146 0.000004026

-------------------------------------------------------------------

Cartesian Forces: Max 0.000944448 RMS 0.000205655

Leave Link 716 at Sat Aug 17 17:48:14 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000736752 RMS 0.000151567

Search for a local minimum.

Step number 39 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .15157D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 4 5 6 2 8

9 10 11 12 13

14 15 16 17 18

20 21 22 23 24

19 26 30 31 27

34 35 33 37 38

39

DE= 3.48D-06 DEPred=-2.11D-05 R=-1.65D-01

Trust test=-1.65D-01 RLast= 1.33D-01 DXMaxT set to 5.00D-02

ITU= -1 -1 0 -1 -1 -1 0 -1 0 0 -1 -1 0 0 -1 0 0 -1 1 -1

ITU= 1 -1 1 1 -1 1 -1 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Eigenvalues --- 0.00074 0.00235 0.00276 0.00299 0.00333

Eigenvalues --- 0.00413 0.00630 0.01267 0.01448 0.02286

Eigenvalues --- 0.03213 0.03550 0.03617 0.04183 0.04580

Eigenvalues --- 0.04798 0.04807 0.04925 0.05405 0.05454

Eigenvalues --- 0.05491 0.05594 0.05762 0.05863 0.08227

Eigenvalues --- 0.08327 0.08549 0.10991 0.11969 0.12205

Eigenvalues --- 0.13392 0.14346 0.15703 0.15953 0.16003

Eigenvalues --- 0.16042 0.16156 0.16241 0.17040 0.17808

Eigenvalues --- 0.19752 0.20331 0.21868 0.22214 0.23270

Eigenvalues --- 0.24450 0.25082 0.25642 0.26415 0.26767

Eigenvalues --- 0.27939 0.28479 0.29118 0.29449 0.29648

Eigenvalues --- 0.30354 0.32148 0.33347 0.33867 0.33880

Eigenvalues --- 0.33915 0.33932 0.33965 0.34020 0.34056

Eigenvalues --- 0.34141 0.34220 0.34424 0.34653 0.34780

Eigenvalues --- 0.35028 0.35870 0.52376 0.56242 0.86408

En-DIIS/RFO-DIIS IScMMF= 0 using points: 39 38 37

RFO step: Lambda=-7.27052085D-06.

NNeg= 0 NP= 3 Switch= 2.50D-03 Rises=F DC= -1.82D-05 SmlDif= 1.00D-05

RMS Error= 0.5063715218D-03 NUsed= 3 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.46697 0.34976 0.18327

Iteration 1 RMS(Cart)= 0.02102916 RMS(Int)= 0.00011921

Iteration 2 RMS(Cart)= 0.00022736 RMS(Int)= 0.00000339

Iteration 3 RMS(Cart)= 0.00000002 RMS(Int)= 0.00000339

ITry= 1 IFail=0 DXMaxC= 6.51D-02 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83555 -0.00028 -0.00015 0.00030 0.00014 2.83569

R2 2.28874 0.00074 -0.00026 0.00056 0.00030 2.28904

R3 2.55343 0.00008 -0.00041 0.00013 -0.00029 2.55314

R4 2.86455 0.00006 0.00085 -0.00028 0.00057 2.86512

R5 3.61583 0.00009 -0.00552 0.00015 -0.00537 3.61046

R6 2.05830 0.00005 -0.00016 0.00021 0.00005 2.05836

R7 1.83680 0.00004 -0.00010 0.00023 0.00013 1.83693

R8 2.06113 0.00001 -0.00007 0.00032 0.00025 2.06138

R9 2.06830 0.00006 -0.00002 0.00022 0.00020 2.06851

R10 2.06010 0.00000 -0.00009 0.00014 0.00004 2.06015

R11 3.31280 0.00007 0.00242 -0.00053 0.00190 3.31469

R12 3.38915 -0.00029 -0.00149 -0.00019 -0.00168 3.38747

R13 3.25223 0.00026 0.00041 0.00081 0.00122 3.25345

R14 3.47151 0.00012 0.00100 0.00050 0.00150 3.47302

R15 2.88112 0.00006 -0.00017 0.00021 0.00004 2.88115

R16 2.06423 -0.00001 -0.00014 0.00008 -0.00006 2.06417

R17 2.05999 0.00006 -0.00009 0.00019 0.00010 2.06009

R18 2.89397 0.00006 -0.00003 0.00012 0.00009 2.89406

R19 2.07193 0.00008 0.00004 0.00011 0.00016 2.07209

R20 2.07114 0.00002 -0.00010 0.00009 -0.00001 2.07114

R21 2.88648 -0.00009 -0.00031 0.00008 -0.00023 2.88625

R22 2.07163 0.00011 0.00005 0.00016 0.00021 2.07184

R23 2.07182 0.00000 -0.00011 0.00008 -0.00003 2.07178

R24 2.06752 0.00004 -0.00008 0.00015 0.00007 2.06760

R25 2.06889 0.00011 0.00005 0.00013 0.00019 2.06908

R26 2.06907 0.00001 -0.00013 0.00011 -0.00002 2.06906

A1 2.17707 -0.00029 0.00015 -0.00063 -0.00047 2.17660

A2 1.97702 0.00005 -0.00039 0.00047 0.00009 1.97711

A3 2.12825 0.00025 0.00052 0.00013 0.00067 2.12892

A4 2.02995 -0.00010 -0.00258 0.00073 -0.00185 2.02810

A5 1.82608 -0.00029 0.00372 -0.00235 0.00137 1.82745

A6 1.87629 -0.00002 -0.00134 -0.00072 -0.00205 1.87423

A7 1.94562 0.00036 0.00060 0.00110 0.00170 1.94732

A8 1.94107 0.00002 -0.00039 0.00095 0.00056 1.94162

A9 1.83093 0.00001 0.00041 0.00003 0.00044 1.83136

A10 1.87241 -0.00006 -0.00026 -0.00030 -0.00057 1.87184

A11 1.91334 0.00004 -0.00031 0.00055 0.00024 1.91358

A12 1.92686 -0.00008 0.00040 -0.00056 -0.00015 1.92671

A13 1.95209 0.00004 -0.00013 0.00005 -0.00008 1.95201

A14 1.88372 0.00000 0.00013 -0.00024 -0.00011 1.88361

A15 1.89380 0.00000 -0.00003 0.00022 0.00019 1.89399

A16 1.89241 0.00000 -0.00006 -0.00002 -0.00008 1.89233

A17 1.80105 0.00021 -0.00233 0.00043 -0.00190 1.79915

A18 1.96906 0.00049 0.00057 0.00105 0.00160 1.97066

A19 2.14395 0.00004 -0.00095 -0.00045 -0.00141 2.14254

A20 2.15755 -0.00058 -0.00078 -0.00164 -0.00243 2.15512

A21 1.79707 -0.00038 -0.00065 -0.00127 -0.00192 1.79516

A22 1.92623 0.00023 0.00008 0.00090 0.00097 1.92720

A23 1.88128 -0.00025 -0.00141 -0.00065 -0.00206 1.87922

A24 1.89084 0.00007 0.00064 0.00029 0.00092 1.89177

A25 1.93915 0.00005 0.00007 -0.00024 -0.00017 1.93897

A26 1.93795 -0.00015 0.00047 -0.00027 0.00020 1.93816

A27 1.88656 0.00002 0.00012 -0.00005 0.00007 1.88663

A28 1.95331 -0.00018 -0.00007 -0.00050 -0.00057 1.95274

A29 1.91590 0.00003 0.00028 0.00003 0.00030 1.91620

A30 1.91773 0.00005 -0.00054 0.00012 -0.00042 1.91730

A31 1.90703 0.00005 0.00001 -0.00034 -0.00033 1.90671

A32 1.90803 0.00007 0.00030 0.00031 0.00062 1.90864

A33 1.85944 -0.00001 0.00002 0.00042 0.00044 1.85988

A34 1.96589 0.00010 0.00021 0.00005 0.00026 1.96614

A35 1.90663 -0.00007 -0.00014 -0.00013 -0.00027 1.90636

A36 1.90773 0.00000 -0.00009 -0.00004 -0.00013 1.90760

A37 1.91263 0.00001 0.00012 -0.00024 -0.00012 1.91251

A38 1.91332 -0.00007 -0.00028 0.00017 -0.00011 1.91321

A39 1.85428 0.00003 0.00018 0.00021 0.00039 1.85467

A40 1.94579 -0.00005 -0.00021 -0.00013 -0.00034 1.94546

A41 1.94219 0.00002 -0.00004 0.00002 -0.00002 1.94217

A42 1.94236 0.00007 0.00036 -0.00016 0.00020 1.94256

A43 1.87741 -0.00001 -0.00022 -0.00007 -0.00030 1.87711

A44 1.87650 0.00002 0.00033 0.00013 0.00046 1.87697

A45 1.87621 -0.00005 -0.00023 0.00023 0.00000 1.87620

D1 2.75535 -0.00023 -0.02915 0.00663 -0.02252 2.73283

D2 -1.37335 -0.00005 -0.02719 0.00671 -0.02047 -1.39382

D3 0.56682 -0.00017 -0.02564 0.00542 -0.02021 0.54661

D4 -0.42994 0.00005 -0.02020 0.00581 -0.01439 -0.44433

D5 1.72455 0.00023 -0.01824 0.00589 -0.01234 1.71221

D6 -2.61847 0.00011 -0.01668 0.00460 -0.01208 -2.63054

D7 -3.09405 -0.00017 -0.00668 0.00030 -0.00638 -3.10043

D8 0.00523 0.00008 0.00198 -0.00052 0.00147 0.00670

D9 3.13235 -0.00001 0.01190 -0.00718 0.00472 3.13707

D10 -1.07787 -0.00003 0.01211 -0.00747 0.00464 -1.07322

D11 1.03097 -0.00006 0.01223 -0.00786 0.00438 1.03535

D12 1.04117 0.00016 0.00835 -0.00545 0.00290 1.04407

D13 3.11414 0.00014 0.00856 -0.00574 0.00282 3.11696

D14 -1.06021 0.00011 0.00868 -0.00612 0.00256 -1.05765

D15 -0.99550 -0.00009 0.00771 -0.00678 0.00092 -0.99458

D16 1.07746 -0.00011 0.00792 -0.00707 0.00085 1.07831

D17 -3.09688 -0.00015 0.00804 -0.00746 0.00058 -3.09630

D18 -3.05891 -0.00008 -0.02499 0.00617 -0.01882 -3.07772

D19 -0.85099 -0.00018 -0.02526 0.00614 -0.01912 -0.87011

D20 1.25164 0.00004 -0.02516 0.00789 -0.01726 1.23438

D21 1.82092 -0.00002 0.00500 0.00150 0.00650 1.82742

D22 -1.15606 0.00034 0.01225 0.00834 0.02059 -1.13547

D23 2.58992 0.00006 -0.01165 0.00381 -0.00784 2.58208

D24 -0.71777 -0.00024 -0.01898 -0.00295 -0.02193 -0.73970

D25 -3.02012 -0.00015 -0.00060 -0.00683 -0.00743 -3.02755

D26 -0.89958 -0.00010 -0.00136 -0.00698 -0.00835 -0.90793

D27 1.13790 -0.00016 -0.00164 -0.00723 -0.00887 1.12902

D28 -3.13181 -0.00008 0.00593 0.00120 0.00713 -3.12468

D29 -1.01118 -0.00011 0.00610 0.00045 0.00655 -1.00462

D30 1.02820 -0.00008 0.00597 0.00105 0.00702 1.03523

D31 1.06552 0.00004 0.00761 0.00157 0.00918 1.07470

D32 -3.09703 0.00001 0.00777 0.00083 0.00860 -3.08843

D33 -1.05765 0.00004 0.00765 0.00143 0.00907 -1.04858

D34 -1.03475 0.00008 0.00709 0.00198 0.00907 -1.02568

D35 1.08589 0.00004 0.00726 0.00123 0.00849 1.09438

D36 3.12527 0.00007 0.00714 0.00183 0.00896 3.13423

D37 -3.12805 -0.00007 -0.00270 0.00090 -0.00180 -3.12985

D38 -0.99835 -0.00004 -0.00251 0.00053 -0.00198 -1.00033

D39 1.02378 -0.00004 -0.00242 0.00069 -0.00173 1.02205

D40 1.02940 -0.00002 -0.00302 0.00143 -0.00159 1.02781

D41 -3.12409 0.00000 -0.00282 0.00106 -0.00176 -3.12585

D42 -1.10196 0.00001 -0.00274 0.00122 -0.00152 -1.10348

D43 -0.99931 -0.00008 -0.00323 0.00094 -0.00228 -1.00160

D44 1.13038 -0.00005 -0.00303 0.00057 -0.00246 1.12792

D45 -3.13067 -0.00005 -0.00294 0.00073 -0.00222 -3.13289

D46 -3.14138 0.00000 -0.00339 0.00312 -0.00028 3.14153

D47 -1.04535 -0.00004 -0.00385 0.00295 -0.00090 -1.04625

D48 1.04682 -0.00004 -0.00392 0.00315 -0.00078 1.04605

D49 1.01551 0.00002 -0.00344 0.00342 -0.00002 1.01549

D50 3.11153 -0.00002 -0.00389 0.00326 -0.00064 3.11090

D51 -1.07948 -0.00002 -0.00397 0.00345 -0.00052 -1.07999

D52 -1.01318 0.00001 -0.00357 0.00322 -0.00035 -1.01354

D53 1.08284 -0.00003 -0.00403 0.00305 -0.00097 1.08187

D54 -3.10817 -0.00003 -0.00410 0.00325 -0.00085 -3.10902

Item Value Threshold Converged?

Maximum Force 0.000737 0.000450 NO

RMS Force 0.000152 0.000300 YES

Maximum Displacement 0.065149 0.001800 NO

RMS Displacement 0.021035 0.001200 NO

Predicted change in Energy=-1.592589D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:48:14 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.089904 -0.412380 -0.219430

2 6 0 -2.848813 0.077523 0.467184

3 8 0 -4.873478 0.294085 -0.814567

4 8 0 -4.243168 -1.753069 -0.152805

5 6 0 -2.309034 -0.799255 1.580121

6 16 0 -1.571816 0.296029 -0.937035

7 6 0 -0.114599 0.762754 -0.079472

8 16 0 1.084138 -0.565234 0.033676

9 16 0 0.019312 2.240072 0.794413

10 6 0 2.689296 0.329393 0.005833

11 6 0 3.847916 -0.658904 -0.067614

12 6 0 5.204774 0.051265 -0.068591

13 6 0 6.378186 -0.922296 -0.158304

14 1 0 -3.050510 1.087166 0.822676

15 1 0 -5.046196 -1.976590 -0.652897

16 1 0 -1.408868 -0.347396 1.998991

17 1 0 -3.045557 -0.890997 2.384658

18 1 0 -2.060999 -1.799471 1.224394

19 1 0 2.683649 0.993706 -0.861231

20 1 0 2.755755 0.944618 0.903339

21 1 0 3.801756 -1.348979 0.783256

22 1 0 3.757862 -1.271489 -0.971961

23 1 0 5.244407 0.752954 -0.910069

24 1 0 5.297480 0.656704 0.840701

25 1 0 7.336881 -0.395024 -0.157631

26 1 0 6.383175 -1.617573 0.687502

27 1 0 6.330517 -1.519251 -1.074912

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.500583 0.000000

3 O 1.211309 2.406044 0.000000

4 O 1.351065 2.383208 2.241888 0.000000

5 C 2.561163 1.516156 3.675091 2.766527 0.000000

6 S 2.712484 1.910575 3.303933 3.456869 2.842396

7 C 4.147720 2.871290 4.838072 4.835269 3.163806

8 S 5.182484 4.008637 6.078744 5.461311 3.736292

9 S 4.994901 3.606916 5.505912 5.917021 3.908458

10 C 6.823381 5.562997 7.607223 7.240226 5.360553

11 C 7.943098 6.758293 8.805046 8.165176 6.375168

12 C 9.307458 8.071432 10.108739 9.619061 7.739441

13 C 10.480680 9.302064 11.336234 10.653796 8.860308

14 H 2.101181 1.089236 2.575413 3.231243 2.163814

15 H 1.883917 3.209743 2.282966 0.972064 3.723513

16 H 3.480455 2.144861 4.509004 3.826146 1.090837

17 H 2.846226 2.157184 3.870497 2.935329 1.094606

18 H 2.850457 2.171895 4.055907 2.580832 1.090182

19 H 6.947663 5.763005 7.589586 7.485148 5.839674

20 H 7.068600 5.687994 7.847266 7.574819 5.399187

21 H 8.010049 6.809176 8.972868 8.109272 6.186998

22 H 7.930435 6.894862 8.773586 8.057258 6.598739

23 H 9.432092 8.237308 10.128735 9.842138 8.103387

24 H 9.507355 8.175394 10.311149 9.890300 7.779822

25 H 11.426965 10.215775 12.247420 11.659410 9.809529

26 H 10.581135 9.388904 11.516201 10.660378 8.776157

27 H 10.513905 9.443932 11.352774 10.616392 9.066943

6 7 8 9 10

6 S 0.000000

7 C 1.754061 0.000000

8 S 2.956035 1.792574 0.000000

9 S 3.051050 1.721649 3.095532 0.000000

10 C 4.364309 2.838468 1.837842 3.376591 0.000000

11 C 5.571471 4.209843 2.767219 4.879074 1.524640

12 C 6.836394 5.366755 4.167754 5.694267 2.531902

13 C 8.080425 6.708343 5.309547 7.165439 3.898920

14 H 2.430847 3.088477 4.521975 3.279299 5.846950

15 H 4.161351 5.670403 6.328057 6.747912 8.098723

16 H 3.010115 2.688415 3.181980 3.191504 4.607132

17 H 3.822903 4.171012 4.763153 4.661104 6.327456

18 H 3.049950 3.471820 3.582323 4.564043 5.346237

19 H 4.312944 2.914563 2.406156 3.375393 1.092311

20 H 4.747159 3.039395 2.414595 3.029552 1.090154

21 H 5.877136 4.532278 2.926016 5.214239 2.158445

22 H 5.555520 4.464373 2.942601 5.424748 2.158874

23 H 6.831574 5.423000 4.464987 5.693716 2.747157

24 H 7.104764 5.490771 4.460569 5.510740 2.758036

25 H 8.969387 7.541293 6.257984 7.835620 4.706543

26 H 8.341636 6.962419 5.441940 7.442555 4.230851

27 H 8.109323 6.909267 5.446431 7.580119 4.224215

11 12 13 14 15

11 C 0.000000

12 C 1.531472 0.000000

13 C 2.545558 1.527339 0.000000

14 H 7.171448 8.367626 9.690231 0.000000

15 H 9.010221 10.465945 11.483582 3.942927 0.000000

16 H 5.657002 6.940756 8.100780 2.477230 4.787164

17 H 7.320347 8.658768 9.760869 2.520503 3.795762

18 H 6.155116 7.608449 8.596576 3.077854 3.530863

19 H 2.171743 2.805805 4.220755 5.977028 8.283512

20 H 2.169528 2.782161 4.211230 5.808575 8.475009

21 H 1.096501 2.157496 2.776074 7.272544 8.985693

22 H 1.095998 2.158544 2.765876 7.425490 8.838009

23 H 2.157142 1.096368 2.158024 8.480552 10.649556

24 H 2.158031 1.096341 2.158513 8.359101 10.777602

25 H 3.500087 2.180133 1.094126 10.538301 12.493488

26 H 2.813679 2.178378 1.094908 9.814699 11.513301

27 H 2.813922 2.178647 1.094897 9.919573 11.393720

16 17 18 19 20

16 H 0.000000

17 H 1.767199 0.000000

18 H 1.770254 1.772257 0.000000

19 H 5.169925 6.849212 5.887559 0.000000

20 H 4.495981 6.262509 5.552857 1.766724 0.000000

21 H 5.443508 7.046980 5.896561 3.072893 2.523712

22 H 6.031219 7.595931 6.241945 2.509443 3.071172

23 H 7.344350 9.070904 8.027438 2.572514 3.085218

24 H 6.879314 8.624701 7.767061 3.137237 2.558747

25 H 9.007853 10.700666 9.602219 4.906749 4.889480

26 H 8.003081 9.607771 8.463180 4.785797 4.446301

27 H 8.409531 10.013696 8.705336 4.433989 4.771064

21 22 23 24 25

21 H 0.000000

22 H 1.757475 0.000000

23 H 3.060509 2.512372 0.000000

24 H 2.502650 3.061715 1.754217 0.000000

25 H 3.780530 3.773685 2.502491 2.502390 0.000000

26 H 2.597122 3.125038 3.077081 2.524786 1.765908

27 H 3.142677 2.586608 2.523831 3.077584 1.765803

26 27

26 H 0.000000

27 H 1.765940 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 2.86D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.100884 -0.470669 -0.139166

2 6 0 -2.853827 0.129505 0.440824

3 8 0 -4.888866 0.122033 -0.842769

4 8 0 -4.254509 -1.778523 0.162983

5 6 0 -2.305469 -0.539463 1.686020

6 16 0 -1.588329 0.095440 -0.990138

7 6 0 -0.123756 0.702343 -0.239522

8 16 0 1.074967 -0.587712 0.095359

9 16 0 0.018382 2.309823 0.360378

10 6 0 2.680451 0.284729 -0.101952

11 6 0 3.837749 -0.703576 -0.010067

12 6 0 5.195038 -0.007485 -0.146561

13 6 0 6.367002 -0.984169 -0.073394

14 1 0 -3.051889 1.186296 0.615179

15 1 0 -5.061795 -2.084644 -0.283657

16 1 0 -1.401563 -0.023012 2.011842

17 1 0 -3.035381 -0.487005 2.500046

18 1 0 -2.061065 -1.587114 1.509408

19 1 0 2.668094 0.786554 -1.072087

20 1 0 2.754746 1.047790 0.673066

21 1 0 3.798150 -1.233494 0.949064

22 1 0 3.739805 -1.465188 -0.792094

23 1 0 5.228195 0.535529 -1.098433

24 1 0 5.295669 0.747955 0.641567

25 1 0 7.326030 -0.467001 -0.172969

26 1 0 6.378506 -1.520207 0.881255

27 1 0 6.311352 -1.732637 -0.870575

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3011576 0.1934217 0.1810083

Leave Link 202 at Sat Aug 17 17:48:14 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.3924510250 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0550060240 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.3374450010 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2321

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.19D-10

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 99

GePol: Fraction of low-weight points (<1% of avg) = 4.27%

GePol: Cavity surface area = 309.042 Ang\*\*2

GePol: Cavity volume = 320.318 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057623246 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.3316826764 Hartrees.

Leave Link 301 at Sat Aug 17 17:48:14 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:48:15 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:48:15 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000614 0.000141 -0.000096 Ang= -0.07 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.63015304951

Leave Link 401 at Sat Aug 17 17:48:15 2019, MaxMem= 1342177280 cpu: 7.7

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16161123.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.77D-15 for 2302.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.49D-15 for 2309 1781.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.55D-15 for 2302.

Iteration 1 A^-1\*A deviation from orthogonality is 2.31D-12 for 2237 939.

E= -1658.67604212082

DIIS: error= 1.00D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67604212082 IErMin= 1 ErrMin= 1.00D-03

ErrMax= 1.00D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.19D-03 BMatP= 2.19D-03

IDIUse=3 WtCom= 9.90D-01 WtEn= 1.00D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.428 Goal= None Shift= 0.000

Gap= 0.484 Goal= None Shift= 0.000

GapD= 0.428 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=1.06D-04 MaxDP=3.01D-03 OVMax= 5.89D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.06D-04 CP: 1.00D+00

E= -1658.67697198047 Delta-E= -0.000929859660 Rises=F Damp=F

DIIS: error= 1.29D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67697198047 IErMin= 2 ErrMin= 1.29D-04

ErrMax= 1.29D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.76D-05 BMatP= 2.19D-03

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.29D-03

Coeff-Com: -0.597D-01 0.106D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.597D-01 0.106D+01

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.10D-05 MaxDP=1.18D-03 DE=-9.30D-04 OVMax= 1.86D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.98D-05 CP: 1.00D+00 1.06D+00

E= -1658.67697770210 Delta-E= -0.000005721627 Rises=F Damp=F

DIIS: error= 2.76D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67697770210 IErMin= 2 ErrMin= 1.29D-04

ErrMax= 2.76D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.82D-05 BMatP= 3.76D-05

IDIUse=3 WtCom= 9.97D-01 WtEn= 2.76D-03

Coeff-Com: -0.399D-01 0.570D+00 0.470D+00

Coeff-En: 0.000D+00 0.217D+00 0.783D+00

Coeff: -0.398D-01 0.569D+00 0.471D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.08D-05 MaxDP=5.15D-04 DE=-5.72D-06 OVMax= 1.09D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 6.84D-06 CP: 1.00D+00 1.09D+00 5.98D-01

E= -1658.67698384120 Delta-E= -0.000006139095 Rises=F Damp=F

DIIS: error= 1.30D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67698384120 IErMin= 2 ErrMin= 1.29D-04

ErrMax= 1.30D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.83D-06 BMatP= 3.76D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.30D-03

Coeff-Com: -0.138D-01 0.179D+00 0.313D+00 0.522D+00

Coeff-En: 0.000D+00 0.000D+00 0.176D+00 0.824D+00

Coeff: -0.138D-01 0.179D+00 0.313D+00 0.522D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.96D-06 MaxDP=1.56D-04 DE=-6.14D-06 OVMax= 3.79D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.95D-06 CP: 1.00D+00 1.10D+00 6.62D-01 6.92D-01

E= -1658.67698525473 Delta-E= -0.000001413536 Rises=F Damp=F

DIIS: error= 1.55D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67698525473 IErMin= 5 ErrMin= 1.55D-05

ErrMax= 1.55D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.31D-07 BMatP= 7.83D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.346D-02 0.386D-01 0.115D+00 0.256D+00 0.594D+00

Coeff: -0.346D-02 0.386D-01 0.115D+00 0.256D+00 0.594D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.18D-06 MaxDP=5.15D-05 DE=-1.41D-06 OVMax= 1.19D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 8.36D-07 CP: 1.00D+00 1.10D+00 6.97D-01 7.47D-01 9.10D-01

E= -1658.67698532569 Delta-E= -0.000000070961 Rises=F Damp=F

DIIS: error= 5.52D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67698532569 IErMin= 6 ErrMin= 5.52D-06

ErrMax= 5.52D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.10D-08 BMatP= 3.31D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.465D-03-0.107D-01 0.810D-02 0.497D-01 0.287D+00 0.665D+00

Coeff: 0.465D-03-0.107D-01 0.810D-02 0.497D-01 0.287D+00 0.665D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.07D-07 MaxDP=2.71D-05 DE=-7.10D-08 OVMax= 5.27D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 3.42D-07 CP: 1.00D+00 1.10D+00 7.11D-01 7.77D-01 9.57D-01

CP: 9.37D-01

E= -1658.67698533629 Delta-E= -0.000000010597 Rises=F Damp=F

DIIS: error= 1.59D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67698533629 IErMin= 7 ErrMin= 1.59D-06

ErrMax= 1.59D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.61D-09 BMatP= 4.10D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.600D-03-0.917D-02-0.102D-01-0.858D-02 0.488D-01 0.281D+00

Coeff-Com: 0.698D+00

Coeff: 0.600D-03-0.917D-02-0.102D-01-0.858D-02 0.488D-01 0.281D+00

Coeff: 0.698D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.74D-07 MaxDP=1.09D-05 DE=-1.06D-08 OVMax= 4.33D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.67D-07 CP: 1.00D+00 1.10D+00 7.14D-01 7.84D-01 1.01D+00

CP: 1.06D+00 1.10D+00

E= -1658.67698533796 Delta-E= -0.000000001668 Rises=F Damp=F

DIIS: error= 6.89D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67698533796 IErMin= 8 ErrMin= 6.89D-07

ErrMax= 6.89D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.05D-09 BMatP= 4.61D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.179D-03-0.205D-02-0.589D-02-0.118D-01-0.264D-01 0.721D-02

Coeff-Com: 0.322D+00 0.717D+00

Coeff: 0.179D-03-0.205D-02-0.589D-02-0.118D-01-0.264D-01 0.721D-02

Coeff: 0.322D+00 0.717D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.28D-07 MaxDP=5.46D-06 DE=-1.67D-09 OVMax= 1.54D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 6.52D-08 CP: 1.00D+00 1.10D+00 7.16D-01 7.89D-01 1.02D+00

CP: 1.14D+00 1.27D+00 8.64D-01

E= -1658.67698533838 Delta-E= -0.000000000419 Rises=F Damp=F

DIIS: error= 3.85D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67698533838 IErMin= 9 ErrMin= 3.85D-07

ErrMax= 3.85D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.26D-10 BMatP= 1.05D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.357D-04 0.106D-02-0.126D-02-0.552D-02-0.294D-01-0.667D-01

Coeff-Com: 0.320D-01 0.462D+00 0.607D+00

Coeff: -0.357D-04 0.106D-02-0.126D-02-0.552D-02-0.294D-01-0.667D-01

Coeff: 0.320D-01 0.462D+00 0.607D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=7.75D-08 MaxDP=3.68D-06 DE=-4.19D-10 OVMax= 1.10D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 2.97D-08 CP: 1.00D+00 1.10D+00 7.18D-01 7.90D-01 1.03D+00

CP: 1.17D+00 1.36D+00 1.11D+00 7.78D-01

E= -1658.67698533851 Delta-E= -0.000000000135 Rises=F Damp=F

DIIS: error= 1.80D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67698533851 IErMin=10 ErrMin= 1.80D-07

ErrMax= 1.80D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.39D-11 BMatP= 4.26D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.560D-04 0.105D-02 0.377D-03-0.113D-02-0.125D-01-0.430D-01

Coeff-Com: -0.506D-01 0.139D+00 0.356D+00 0.611D+00

Coeff: -0.560D-04 0.105D-02 0.377D-03-0.113D-02-0.125D-01-0.430D-01

Coeff: -0.506D-01 0.139D+00 0.356D+00 0.611D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.31D-08 MaxDP=1.29D-06 DE=-1.35D-10 OVMax= 3.25D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.27D-08 CP: 1.00D+00 1.10D+00 7.18D-01 7.91D-01 1.03D+00

CP: 1.17D+00 1.40D+00 1.14D+00 8.93D-01 8.36D-01

E= -1658.67698533854 Delta-E= -0.000000000029 Rises=F Damp=F

DIIS: error= 5.98D-08 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67698533854 IErMin=11 ErrMin= 5.98D-08

ErrMax= 5.98D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.05D-12 BMatP= 7.39D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.164D-04 0.237D-03 0.341D-03 0.395D-03-0.353D-04-0.573D-02

Coeff-Com: -0.242D-01-0.132D-01 0.410D-01 0.272D+00 0.729D+00

Coeff: -0.164D-04 0.237D-03 0.341D-03 0.395D-03-0.353D-04-0.573D-02

Coeff: -0.242D-01-0.132D-01 0.410D-01 0.272D+00 0.729D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.01D-08 MaxDP=4.58D-07 DE=-2.91D-11 OVMax= 1.29D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 5.48D-09 CP: 1.00D+00 1.10D+00 7.18D-01 7.91D-01 1.03D+00

CP: 1.18D+00 1.40D+00 1.17D+00 9.23D-01 9.78D-01

CP: 9.86D-01

E= -1658.67698533857 Delta-E= -0.000000000028 Rises=F Damp=F

DIIS: error= 3.90D-08 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.67698533857 IErMin=12 ErrMin= 3.90D-08

ErrMax= 3.90D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.82D-12 BMatP= 8.05D-12

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.753D-06-0.558D-04 0.110D-03 0.388D-03 0.210D-02 0.436D-02

Coeff-Com: -0.497D-02-0.320D-01-0.445D-01 0.410D-01 0.385D+00 0.649D+00

Coeff: 0.753D-06-0.558D-04 0.110D-03 0.388D-03 0.210D-02 0.436D-02

Coeff: -0.497D-02-0.320D-01-0.445D-01 0.410D-01 0.385D+00 0.649D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.95D-09 MaxDP=2.13D-07 DE=-2.77D-11 OVMax= 3.50D-07

Error on total polarization charges = 0.04163

SCF Done: E(UB3LYP) = -1658.67698534 A.U. after 12 cycles

NFock= 12 Conv=0.40D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655237368221D+03 PE=-6.147432653218D+03 EE= 1.731186616982D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.62

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:48:42 2019, MaxMem= 1342177280 cpu: 302.9

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 337

Leave Link 701 at Sat Aug 17 17:48:43 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:48:43 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:48:46 2019, MaxMem= 1342177280 cpu: 38.3

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.39850846D+00-2.92992407D+00 6.49751046D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000140300 -0.000192533 0.000290359

2 6 0.000006238 0.000164630 0.000057069

3 8 -0.000105216 0.000237542 -0.000147368

4 8 0.000011665 -0.000017374 -0.000096598

5 6 0.000044746 -0.000118373 -0.000067690

6 16 -0.000024409 -0.000028275 -0.000073539

7 6 0.000053913 -0.000077688 -0.000036732

8 16 0.000068416 0.000057194 -0.000027849

9 16 0.000036165 0.000064654 0.000114984

10 6 -0.000048202 0.000033684 0.000104699

11 6 0.000003312 -0.000020646 -0.000019765

12 6 0.000018261 0.000012646 -0.000001888

13 6 -0.000032682 0.000049478 -0.000055801

14 1 -0.000048519 -0.000073390 0.000090506

15 1 -0.000025385 -0.000008026 -0.000031760

16 1 -0.000059087 -0.000012078 -0.000038135

17 1 -0.000016465 -0.000021387 -0.000007688

18 1 -0.000013677 -0.000030587 -0.000004397

19 1 -0.000030736 0.000025399 -0.000010131

20 1 0.000012285 -0.000018598 0.000035866

21 1 -0.000020874 -0.000054285 -0.000013664

22 1 -0.000020095 0.000033967 -0.000051606

23 1 -0.000008488 0.000063536 -0.000000405

24 1 0.000027204 -0.000035670 0.000033898

25 1 0.000020766 0.000012087 -0.000003228

26 1 0.000019901 -0.000054502 -0.000012240

27 1 -0.000009338 0.000008596 -0.000026893

-------------------------------------------------------------------

Cartesian Forces: Max 0.000290359 RMS 0.000070810

Leave Link 716 at Sat Aug 17 17:48:46 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000271910 RMS 0.000043140

Search for a local minimum.

Step number 40 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .43140D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40

DE= -1.04D-05 DEPred=-1.59D-05 R= 6.54D-01

TightC=F SS= 1.41D+00 RLast= 7.03D-02 DXNew= 8.4090D-02 2.1078D-01

Trust test= 6.54D-01 RLast= 7.03D-02 DXMaxT set to 8.41D-02

ITU= 1 -1 -1 0 -1 -1 -1 0 -1 0 0 -1 -1 0 0 -1 0 0 -1 1

ITU= -1 1 -1 1 1 -1 1 -1 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Eigenvalues --- 0.00083 0.00253 0.00283 0.00307 0.00336

Eigenvalues --- 0.00402 0.00635 0.01374 0.01439 0.02266

Eigenvalues --- 0.03194 0.03535 0.03631 0.04303 0.04542

Eigenvalues --- 0.04710 0.04805 0.04892 0.05372 0.05458

Eigenvalues --- 0.05486 0.05605 0.05702 0.05902 0.08230

Eigenvalues --- 0.08335 0.08632 0.11016 0.11974 0.12199

Eigenvalues --- 0.13553 0.14648 0.15642 0.15959 0.15977

Eigenvalues --- 0.16045 0.16160 0.16236 0.16977 0.17992

Eigenvalues --- 0.19877 0.21090 0.21912 0.22315 0.23291

Eigenvalues --- 0.24392 0.25067 0.25540 0.26032 0.26679

Eigenvalues --- 0.28013 0.28224 0.29076 0.29513 0.29617

Eigenvalues --- 0.30477 0.32039 0.32919 0.33628 0.33880

Eigenvalues --- 0.33913 0.33927 0.33940 0.34016 0.34038

Eigenvalues --- 0.34111 0.34225 0.34308 0.34699 0.34771

Eigenvalues --- 0.34868 0.35825 0.52471 0.56484 0.85896

En-DIIS/RFO-DIIS IScMMF= 0 using points: 40 39 38 37

RFO step: Lambda=-5.50660498D-07.

NNeg= 0 NP= 4 Switch= 2.50D-03 Rises=F DC= -1.82D-05 SmlDif= 1.00D-05

RMS Error= 0.1396924290D-03 NUsed= 4 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 0.94241 0.07453 -0.04995 0.03301

Iteration 1 RMS(Cart)= 0.00607196 RMS(Int)= 0.00001435

Iteration 2 RMS(Cart)= 0.00002522 RMS(Int)= 0.00000014

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000014

ITry= 1 IFail=0 DXMaxC= 1.90D-02 DCOld= 1.00D+10 DXMaxT= 8.41D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83569 -0.00003 0.00012 -0.00048 -0.00036 2.83533

R2 2.28904 0.00027 -0.00009 0.00070 0.00060 2.28965

R3 2.55314 0.00006 0.00005 0.00005 0.00009 2.55324

R4 2.86512 -0.00005 -0.00008 -0.00002 -0.00010 2.86502

R5 3.61046 0.00011 0.00018 0.00069 0.00087 3.61133

R6 2.05836 -0.00003 -0.00002 0.00006 0.00004 2.05840

R7 1.83693 0.00002 -0.00001 0.00012 0.00011 1.83704

R8 2.06138 -0.00005 -0.00002 -0.00006 -0.00007 2.06131

R9 2.06851 0.00001 -0.00001 0.00008 0.00007 2.06858

R10 2.06015 -0.00001 0.00001 -0.00003 -0.00002 2.06012

R11 3.31469 0.00009 -0.00009 0.00022 0.00013 3.31483

R12 3.38747 -0.00003 0.00003 0.00002 0.00005 3.38753

R13 3.25345 0.00009 -0.00004 0.00046 0.00042 3.25386

R14 3.47302 -0.00006 -0.00001 -0.00038 -0.00039 3.47263

R15 2.88115 0.00003 -0.00001 0.00014 0.00013 2.88128

R16 2.06417 0.00003 -0.00001 0.00012 0.00011 2.06428

R17 2.06009 0.00001 0.00000 0.00002 0.00002 2.06011

R18 2.89406 0.00004 0.00000 0.00020 0.00019 2.89426

R19 2.07209 0.00004 -0.00001 0.00015 0.00015 2.07223

R20 2.07114 0.00002 -0.00001 0.00009 0.00008 2.07122

R21 2.88625 0.00001 0.00001 -0.00007 -0.00006 2.88620

R22 2.07184 0.00004 -0.00002 0.00020 0.00018 2.07202

R23 2.07178 0.00001 0.00000 0.00003 0.00003 2.07182

R24 2.06760 0.00002 0.00000 0.00008 0.00009 2.06768

R25 2.06908 0.00005 -0.00002 0.00021 0.00020 2.06927

R26 2.06906 0.00000 0.00000 0.00002 0.00002 2.06908

A1 2.17660 -0.00012 0.00001 -0.00065 -0.00064 2.17596

A2 1.97711 0.00008 -0.00003 0.00043 0.00040 1.97751

A3 2.12892 0.00004 -0.00001 0.00022 0.00021 2.12912

A4 2.02810 -0.00001 0.00012 -0.00013 -0.00001 2.02809

A5 1.82745 -0.00003 -0.00011 -0.00034 -0.00046 1.82699

A6 1.87423 0.00001 0.00008 -0.00028 -0.00021 1.87403

A7 1.94732 0.00002 -0.00013 0.00053 0.00040 1.94772

A8 1.94162 -0.00003 -0.00003 -0.00018 -0.00021 1.94142

A9 1.83136 0.00004 0.00007 0.00044 0.00051 1.83188

A10 1.87184 0.00006 0.00013 -0.00006 0.00006 1.87191

A11 1.91358 -0.00008 -0.00004 -0.00049 -0.00052 1.91306

A12 1.92671 -0.00005 0.00002 -0.00042 -0.00040 1.92631

A13 1.95201 0.00007 0.00005 0.00052 0.00058 1.95259

A14 1.88361 0.00003 -0.00001 -0.00013 -0.00014 1.88347

A15 1.89399 0.00003 -0.00002 0.00036 0.00034 1.89433

A16 1.89233 0.00000 -0.00001 0.00016 0.00015 1.89248

A17 1.79915 0.00007 0.00012 0.00020 0.00033 1.79948

A18 1.97066 0.00001 0.00000 -0.00014 -0.00014 1.97052

A19 2.14254 0.00003 0.00011 -0.00028 -0.00017 2.14237

A20 2.15512 -0.00004 0.00005 -0.00037 -0.00032 2.15480

A21 1.79516 0.00006 0.00003 0.00008 0.00012 1.79527

A22 1.92720 -0.00010 -0.00002 -0.00016 -0.00018 1.92702

A23 1.87922 0.00001 0.00001 -0.00057 -0.00056 1.87866

A24 1.89177 0.00004 0.00005 0.00021 0.00025 1.89202

A25 1.93897 0.00001 0.00000 -0.00014 -0.00014 1.93884

A26 1.93816 0.00003 -0.00004 0.00047 0.00043 1.93858

A27 1.88663 0.00000 0.00000 0.00018 0.00018 1.88680

A28 1.95274 0.00004 0.00004 -0.00019 -0.00014 1.95260

A29 1.91620 -0.00001 0.00003 0.00010 0.00013 1.91633

A30 1.91730 -0.00003 -0.00003 -0.00021 -0.00024 1.91707

A31 1.90671 0.00000 -0.00002 0.00025 0.00023 1.90694

A32 1.90864 0.00000 0.00001 0.00000 0.00001 1.90865

A33 1.85988 0.00000 -0.00004 0.00006 0.00002 1.85990

A34 1.96614 -0.00001 -0.00001 0.00008 0.00007 1.96622

A35 1.90636 -0.00001 0.00002 -0.00009 -0.00007 1.90629

A36 1.90760 0.00002 0.00001 0.00005 0.00006 1.90766

A37 1.91251 0.00002 -0.00001 0.00023 0.00022 1.91273

A38 1.91321 -0.00002 0.00003 -0.00042 -0.00038 1.91282

A39 1.85467 0.00000 -0.00005 0.00015 0.00010 1.85476

A40 1.94546 0.00000 0.00004 -0.00015 -0.00011 1.94535

A41 1.94217 0.00003 0.00003 0.00002 0.00005 1.94222

A42 1.94256 0.00001 -0.00001 0.00022 0.00022 1.94278

A43 1.87711 -0.00002 -0.00001 -0.00008 -0.00009 1.87703

A44 1.87697 0.00000 -0.00006 0.00028 0.00022 1.87718

A45 1.87620 -0.00002 0.00000 -0.00030 -0.00030 1.87590

D1 2.73283 0.00001 0.00126 0.00070 0.00196 2.73478

D2 -1.39382 0.00001 0.00108 0.00104 0.00212 -1.39170

D3 0.54661 0.00005 0.00114 0.00127 0.00241 0.54902

D4 -0.44433 -0.00004 0.00020 0.00079 0.00099 -0.44334

D5 1.71221 -0.00004 0.00002 0.00113 0.00115 1.71336

D6 -2.63054 0.00000 0.00008 0.00136 0.00144 -2.62910

D7 -3.10043 0.00002 0.00069 -0.00076 -0.00007 -3.10050

D8 0.00670 -0.00004 -0.00033 -0.00070 -0.00103 0.00567

D9 3.13707 0.00001 -0.00053 0.00025 -0.00029 3.13679

D10 -1.07322 -0.00003 -0.00056 -0.00048 -0.00103 -1.07426

D11 1.03535 -0.00001 -0.00052 -0.00022 -0.00074 1.03461

D12 1.04407 0.00005 -0.00037 0.00038 0.00001 1.04408

D13 3.11696 0.00001 -0.00039 -0.00034 -0.00074 3.11623

D14 -1.05765 0.00002 -0.00036 -0.00008 -0.00044 -1.05809

D15 -0.99458 -0.00001 -0.00036 -0.00039 -0.00075 -0.99533

D16 1.07831 -0.00005 -0.00038 -0.00112 -0.00150 1.07681

D17 -3.09630 -0.00003 -0.00034 -0.00086 -0.00120 -3.09750

D18 -3.07772 0.00001 0.00033 0.00000 0.00034 -3.07738

D19 -0.87011 -0.00001 0.00033 -0.00007 0.00026 -0.86986

D20 1.23438 0.00000 0.00026 0.00028 0.00054 1.23492

D21 1.82742 0.00000 -0.00022 -0.00050 -0.00072 1.82670

D22 -1.13547 0.00002 -0.00119 0.00423 0.00304 -1.13244

D23 2.58208 0.00006 0.00015 0.00469 0.00484 2.58692

D24 -0.73970 0.00005 0.00114 -0.00007 0.00107 -0.73863

D25 -3.02755 0.00005 0.00132 0.00762 0.00894 -3.01861

D26 -0.90793 0.00001 0.00132 0.00699 0.00831 -0.89961

D27 1.12902 0.00004 0.00135 0.00701 0.00836 1.13738

D28 -3.12468 -0.00002 -0.00001 0.00059 0.00058 -3.12410

D29 -1.00462 0.00000 0.00002 0.00085 0.00087 -1.00375

D30 1.03523 -0.00002 -0.00003 0.00087 0.00083 1.03606

D31 1.07470 0.00002 -0.00001 0.00150 0.00149 1.07619

D32 -3.08843 0.00004 0.00001 0.00176 0.00177 -3.08666

D33 -1.04858 0.00002 -0.00004 0.00177 0.00174 -1.04684

D34 -1.02568 -0.00001 0.00002 0.00105 0.00107 -1.02461

D35 1.09438 0.00001 0.00004 0.00131 0.00135 1.09573

D36 3.13423 -0.00001 -0.00001 0.00133 0.00132 3.13554

D37 -3.12985 0.00001 0.00064 -0.00146 -0.00082 -3.13067

D38 -1.00033 0.00002 0.00064 -0.00117 -0.00054 -1.00087

D39 1.02205 0.00002 0.00059 -0.00102 -0.00043 1.02162

D40 1.02781 -0.00001 0.00059 -0.00164 -0.00105 1.02676

D41 -3.12585 0.00000 0.00059 -0.00135 -0.00077 -3.12662

D42 -1.10348 0.00001 0.00054 -0.00120 -0.00065 -1.10413

D43 -1.00160 -0.00001 0.00064 -0.00185 -0.00121 -1.00281

D44 1.12792 0.00000 0.00064 -0.00156 -0.00093 1.12700

D45 -3.13289 0.00000 0.00060 -0.00141 -0.00081 -3.13370

D46 3.14153 0.00000 0.00049 -0.00255 -0.00205 3.13948

D47 -1.04625 -0.00001 0.00053 -0.00273 -0.00220 -1.04845

D48 1.04605 -0.00001 0.00055 -0.00295 -0.00240 1.04364

D49 1.01549 0.00000 0.00047 -0.00265 -0.00218 1.01331

D50 3.11090 0.00000 0.00051 -0.00283 -0.00232 3.10857

D51 -1.07999 -0.00001 0.00053 -0.00305 -0.00253 -1.08252

D52 -1.01354 0.00000 0.00053 -0.00273 -0.00220 -1.01573

D53 1.08187 0.00000 0.00056 -0.00291 -0.00235 1.07953

D54 -3.10902 -0.00001 0.00058 -0.00313 -0.00255 -3.11157

Item Value Threshold Converged?

Maximum Force 0.000272 0.000450 YES

RMS Force 0.000043 0.000300 YES

Maximum Displacement 0.018952 0.001800 NO

RMS Displacement 0.006072 0.001200 NO

Predicted change in Energy=-1.219520D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:48:46 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.089033 -0.415246 -0.220637

2 6 0 -2.848884 0.077790 0.465022

3 8 0 -4.871302 0.289137 -0.820589

4 8 0 -4.242709 -1.755650 -0.148440

5 6 0 -2.309495 -0.794583 1.581534

6 16 0 -1.571321 0.291904 -0.939982

7 6 0 -0.114109 0.762090 -0.084159

8 16 0 1.084389 -0.565669 0.034479

9 16 0 0.017709 2.240784 0.788149

10 6 0 2.689450 0.328849 0.011764

11 6 0 3.847781 -0.659292 -0.069382

12 6 0 5.204856 0.050673 -0.065520

13 6 0 6.378149 -0.922373 -0.161656

14 1 0 -3.051769 1.088452 0.816985

15 1 0 -5.045307 -1.981182 -0.648434

16 1 0 -1.409806 -0.340435 1.998849

17 1 0 -3.046470 -0.882667 2.386117

18 1 0 -2.061161 -1.796336 1.230402

19 1 0 2.682976 0.998563 -0.851202

20 1 0 2.756594 0.938349 0.913127

21 1 0 3.801620 -1.355937 0.776219

22 1 0 3.757159 -1.264854 -0.978442

23 1 0 5.244496 0.758218 -0.902206

24 1 0 5.297838 0.649711 0.847994

25 1 0 7.336818 -0.394966 -0.159466

26 1 0 6.384326 -1.621959 0.680719

27 1 0 6.329363 -1.515005 -1.081021

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.500394 0.000000

3 O 1.211628 2.405750 0.000000

4 O 1.351115 2.383398 2.242335 0.000000

5 C 2.560951 1.516105 3.675255 2.766546 0.000000

6 S 2.712267 1.911034 3.302141 3.457648 2.843132

7 C 4.147862 2.872083 4.837033 4.836164 3.165041

8 S 5.181892 4.008746 6.077178 5.461455 3.736875

9 S 4.993744 3.605595 5.504488 5.916067 3.906251

10 C 6.823161 5.562520 7.606534 7.240555 5.358706

11 C 7.942005 6.758269 8.802626 8.164820 6.376196

12 C 9.306853 8.071242 10.107223 9.619053 7.739039

13 C 10.479625 9.302214 11.333670 10.653504 8.861726

14 H 2.100877 1.089256 2.575121 3.230990 2.163638

15 H 1.884045 3.209894 2.283476 0.972122 3.723633

16 H 3.479938 2.144407 4.508608 3.826098 1.090799

17 H 2.846153 2.156878 3.871188 2.935484 1.094644

18 H 2.850472 2.172248 4.056187 2.581089 1.090171

19 H 6.946695 5.760360 7.587578 7.486300 5.835953

20 H 7.069670 5.688826 7.849333 7.574615 5.395839

21 H 8.008809 6.810405 8.970821 8.107157 6.189457

22 H 7.928356 6.893917 8.768702 8.057771 6.601433

23 H 9.431666 8.236207 10.126997 9.843514 8.102033

24 H 9.507336 8.175747 10.311430 9.889423 7.777891

25 H 11.426033 10.215773 12.245133 11.659204 9.810308

26 H 10.581108 9.390838 11.515006 10.660172 8.779439

27 H 10.511551 9.442853 11.348024 10.615853 9.068522

6 7 8 9 10

6 S 0.000000

7 C 1.754130 0.000000

8 S 2.955977 1.792601 0.000000

9 S 3.051162 1.721869 3.095482 0.000000

10 C 4.365931 2.838459 1.837634 3.375866 0.000000

11 C 5.570402 4.209171 2.766927 4.880087 1.524709

12 C 6.836625 5.366364 4.167508 5.694896 2.531920

13 C 8.079252 6.707670 5.309387 7.166790 3.898990

14 H 2.431697 3.090052 4.522858 3.278780 5.846964

15 H 4.161790 5.671037 6.327971 6.747066 8.099294

16 H 3.010426 2.689482 3.182843 3.188461 4.604384

17 H 3.823430 4.172078 4.763894 4.658180 6.325038

18 H 3.051435 3.473417 3.583191 4.562414 5.345072

19 H 4.313501 2.909977 2.405563 3.366636 1.092369

20 H 4.752130 3.044106 2.414614 3.035366 1.090162

21 H 5.876156 4.534228 2.925413 5.220587 2.158660

22 H 5.551366 4.460377 2.942544 5.421608 2.158795

23 H 6.831855 5.420689 4.465036 5.689869 2.747355

24 H 7.107055 5.492788 4.460057 5.514967 2.757883

25 H 8.968608 7.540608 6.257765 7.836741 4.706512

26 H 8.341574 6.964079 5.442675 7.447559 4.231460

27 H 8.105900 6.906319 5.445671 7.578703 4.224091

11 12 13 14 15

11 C 0.000000

12 C 1.531574 0.000000

13 C 2.545680 1.527310 0.000000

14 H 7.172451 8.368253 9.691466 0.000000

15 H 9.009423 10.465852 11.482742 3.942626 0.000000

16 H 5.658752 6.940342 8.103004 2.476805 4.787173

17 H 7.321889 8.658293 9.762999 2.519428 3.796127

18 H 6.156127 7.608275 8.597882 3.078022 3.531193

19 H 2.171750 2.806362 4.221347 5.973126 8.285310

20 H 2.169901 2.782033 4.211069 5.811098 8.475363

21 H 1.096579 2.157811 2.775984 7.276376 8.982688

22 H 1.096041 2.158672 2.766590 7.424494 8.837728

23 H 2.157254 1.096465 2.158233 8.478956 10.651233

24 H 2.158178 1.096358 2.158220 8.361184 10.776898

25 H 3.500195 2.180065 1.094172 10.539295 12.492886

26 H 2.814861 2.178467 1.095013 9.818594 11.512263

27 H 2.813167 2.178785 1.094909 9.918975 11.392435

16 17 18 19 20

16 H 0.000000

17 H 1.767105 0.000000

18 H 1.770430 1.772372 0.000000

19 H 5.163969 6.844401 5.886542 0.000000

20 H 4.491433 6.257903 5.548866 1.766890 0.000000

21 H 5.448397 7.050680 5.896815 3.073033 2.524791

22 H 6.034595 7.599717 6.246143 2.508608 3.071362

23 H 7.341859 9.068941 8.027851 2.573276 3.085051

24 H 6.877307 8.622151 7.764293 3.137908 2.558413

25 H 9.009148 10.701894 9.602999 4.907002 4.889442

26 H 8.008013 9.612224 8.465152 4.786847 4.446305

27 H 8.411894 10.016344 8.707624 4.434747 4.770771

21 22 23 24 25

21 H 0.000000

22 H 1.757586 0.000000

23 H 3.060825 2.512131 0.000000

24 H 2.503286 3.061881 1.754371 0.000000

25 H 3.781085 3.773776 2.501861 2.502752 0.000000

26 H 2.598126 3.127674 3.077353 2.523672 1.765974

27 H 3.140722 2.586374 2.525164 3.077522 1.765989

26 27

26 H 0.000000

27 H 1.765839 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.53D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.100209 -0.471586 -0.138962

2 6 0 -2.853918 0.130626 0.440071

3 8 0 -4.886862 0.119136 -0.846257

4 8 0 -4.254457 -1.778471 0.167260

5 6 0 -2.305950 -0.534814 1.687266

6 16 0 -1.587998 0.093333 -0.991050

7 6 0 -0.123244 0.702230 -0.242243

8 16 0 1.075036 -0.587255 0.096537

9 16 0 0.017192 2.310130 0.357566

10 6 0 2.680639 0.285834 -0.094926

11 6 0 3.837376 -0.704007 -0.011793

12 6 0 5.195061 -0.007426 -0.142876

13 6 0 6.366647 -0.985053 -0.077257

14 1 0 -3.052951 1.187666 0.611915

15 1 0 -5.061419 -2.085909 -0.279187

16 1 0 -1.402391 -0.016919 2.011625

17 1 0 -3.036226 -0.479446 2.500823

18 1 0 -2.061453 -1.583042 1.514316

19 1 0 2.667515 0.794720 -1.061431

20 1 0 2.755879 1.043094 0.685681

21 1 0 3.797697 -1.242317 0.942740

22 1 0 3.738596 -1.458678 -0.800477

23 1 0 5.228304 0.543189 -1.090480

24 1 0 5.296232 0.741594 0.651313

25 1 0 7.325767 -0.467591 -0.174901

26 1 0 6.379275 -1.526944 0.874188

27 1 0 6.309628 -1.728888 -0.878683

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3006662 0.1934444 0.1810391

Leave Link 202 at Sat Aug 17 17:48:46 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.3977702493 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0550077212 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.3427625281 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2319

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.14D-07

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 95

GePol: Fraction of low-weight points (<1% of avg) = 4.10%

GePol: Cavity surface area = 309.000 Ang\*\*2

GePol: Cavity volume = 320.282 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057643632 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.3369981649 Hartrees.

Leave Link 301 at Sat Aug 17 17:48:46 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:48:46 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:48:46 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000456 0.000022 -0.000021 Ang= 0.05 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 17:48:47 2019, MaxMem= 1342177280 cpu: 2.7

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16133283.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.00D-15 for 2299.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.17D-15 for 2158 155.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.55D-15 for 2299.

Iteration 1 A^-1\*A deviation from orthogonality is 1.64D-12 for 2110 890.

E= -1658.67690109491

DIIS: error= 4.97D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67690109491 IErMin= 1 ErrMin= 4.97D-04

ErrMax= 4.97D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.85D-04 BMatP= 1.85D-04

IDIUse=3 WtCom= 9.95D-01 WtEn= 4.97D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.428 Goal= None Shift= 0.000

Gap= 0.484 Goal= None Shift= 0.000

RMSDP=2.74D-05 MaxDP=5.89D-04 OVMax= 2.61D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.74D-05 CP: 1.00D+00

E= -1658.67698758029 Delta-E= -0.000086485381 Rises=F Damp=F

DIIS: error= 4.44D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67698758029 IErMin= 2 ErrMin= 4.44D-05

ErrMax= 4.44D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.06D-06 BMatP= 1.85D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.713D-01 0.107D+01

Coeff: -0.713D-01 0.107D+01

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.53D-06 MaxDP=1.28D-04 DE=-8.65D-05 OVMax= 3.32D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.18D-06 CP: 1.00D+00 1.12D+00

E= -1658.67698849482 Delta-E= -0.000000914523 Rises=F Damp=F

DIIS: error= 1.91D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67698849482 IErMin= 3 ErrMin= 1.91D-05

ErrMax= 1.91D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.53D-07 BMatP= 2.06D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.282D-01 0.368D+00 0.660D+00

Coeff: -0.282D-01 0.368D+00 0.660D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.52D-06 MaxDP=8.16D-05 DE=-9.15D-07 OVMax= 1.28D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.44D-06 CP: 1.00D+00 1.13D+00 8.95D-01

E= -1658.67698852061 Delta-E= -0.000000025798 Rises=F Damp=F

DIIS: error= 2.33D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67698852061 IErMin= 3 ErrMin= 1.91D-05

ErrMax= 2.33D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.55D-07 BMatP= 4.53D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.948D-02 0.108D+00 0.461D+00 0.440D+00

Coeff: -0.948D-02 0.108D+00 0.461D+00 0.440D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=7.45D-07 MaxDP=4.25D-05 DE=-2.58D-08 OVMax= 7.94D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.38D-07 CP: 1.00D+00 1.13D+00 9.93D-01 6.48D-01

E= -1658.67698858430 Delta-E= -0.000000063684 Rises=F Damp=F

DIIS: error= 4.52D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67698858430 IErMin= 5 ErrMin= 4.52D-06

ErrMax= 4.52D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.16D-08 BMatP= 3.55D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.201D-02 0.172D-01 0.160D+00 0.212D+00 0.613D+00

Coeff: -0.201D-02 0.172D-01 0.160D+00 0.212D+00 0.613D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.24D-07 MaxDP=8.45D-06 DE=-6.37D-08 OVMax= 2.38D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.70D-07 CP: 1.00D+00 1.13D+00 1.03D+00 6.93D-01 8.87D-01

E= -1658.67698858654 Delta-E= -0.000000002241 Rises=F Damp=F

DIIS: error= 1.69D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67698858654 IErMin= 6 ErrMin= 1.69D-06

ErrMax= 1.69D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.50D-09 BMatP= 1.16D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.628D-03-0.111D-01 0.421D-02 0.384D-01 0.347D+00 0.621D+00

Coeff: 0.628D-03-0.111D-01 0.421D-02 0.384D-01 0.347D+00 0.621D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.18D-07 MaxDP=4.87D-06 DE=-2.24D-09 OVMax= 1.47D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 8.04D-08 CP: 1.00D+00 1.14D+00 1.04D+00 7.23D-01 9.97D-01

CP: 1.04D+00

E= -1658.67698858711 Delta-E= -0.000000000574 Rises=F Damp=F

DIIS: error= 4.44D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67698858711 IErMin= 7 ErrMin= 4.44D-07

ErrMax= 4.44D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.03D-10 BMatP= 2.50D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.459D-03-0.634D-02-0.147D-01-0.563D-02 0.869D-01 0.271D+00

Coeff-Com: 0.669D+00

Coeff: 0.459D-03-0.634D-02-0.147D-01-0.563D-02 0.869D-01 0.271D+00

Coeff: 0.669D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.90D-08 MaxDP=2.64D-06 DE=-5.74D-10 OVMax= 5.62D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.83D-08 CP: 1.00D+00 1.14D+00 1.05D+00 7.33D-01 1.05D+00

CP: 1.17D+00 1.08D+00

E= -1658.67698858718 Delta-E= -0.000000000070 Rises=F Damp=F

DIIS: error= 1.58D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67698858718 IErMin= 8 ErrMin= 1.58D-07

ErrMax= 1.58D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.08D-11 BMatP= 2.03D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.536D-04-0.372D-04-0.752D-02-0.115D-01-0.442D-01-0.317D-01

Coeff-Com: 0.299D+00 0.796D+00

Coeff: 0.536D-04-0.372D-04-0.752D-02-0.115D-01-0.442D-01-0.317D-01

Coeff: 0.299D+00 0.796D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.38D-08 MaxDP=1.76D-06 DE=-7.00D-11 OVMax= 5.04D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.04D-08 CP: 1.00D+00 1.14D+00 1.05D+00 7.39D-01 1.07D+00

CP: 1.28D+00 1.28D+00 1.07D+00

E= -1658.67698858720 Delta-E= -0.000000000015 Rises=F Damp=F

DIIS: error= 4.57D-08 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67698858720 IErMin= 9 ErrMin= 4.57D-08

ErrMax= 4.57D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.97D-12 BMatP= 4.08D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.435D-04 0.895D-03-0.938D-03-0.395D-02-0.304D-01-0.542D-01

Coeff-Com: 0.129D-01 0.308D+00 0.768D+00

Coeff: -0.435D-04 0.895D-03-0.938D-03-0.395D-02-0.304D-01-0.542D-01

Coeff: 0.129D-01 0.308D+00 0.768D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.24D-08 MaxDP=7.40D-07 DE=-1.46D-11 OVMax= 1.67D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 4.14D-09 CP: 1.00D+00 1.14D+00 1.06D+00 7.41D-01 1.08D+00

CP: 1.31D+00 1.37D+00 1.22D+00 9.19D-01

E= -1658.67698858721 Delta-E= -0.000000000009 Rises=F Damp=F

DIIS: error= 1.51D-08 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67698858721 IErMin=10 ErrMin= 1.51D-08

ErrMax= 1.51D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.77D-13 BMatP= 4.97D-12

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.216D-04 0.344D-03 0.331D-03-0.500D-03-0.778D-02-0.189D-01

Coeff-Com: -0.260D-01 0.457D-01 0.327D+00 0.680D+00

Coeff: -0.216D-04 0.344D-03 0.331D-03-0.500D-03-0.778D-02-0.189D-01

Coeff: -0.260D-01 0.457D-01 0.327D+00 0.680D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.10D-09 MaxDP=1.53D-07 DE=-9.09D-12 OVMax= 4.10D-07

Error on total polarization charges = 0.04163

SCF Done: E(UB3LYP) = -1658.67698859 A.U. after 10 cycles

NFock= 10 Conv=0.31D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655234921820D+03 PE=-6.147442182116D+03 EE= 1.731193273543D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.62

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:49:09 2019, MaxMem= 1342177280 cpu: 255.2

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 338

Leave Link 701 at Sat Aug 17 17:49:10 2019, MaxMem= 1342177280 cpu: 10.2

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:49:10 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:49:13 2019, MaxMem= 1342177280 cpu: 37.2

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.40081366D+00-2.92811433D+00 6.59465196D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000091237 0.000062326 -0.000058537

2 6 -0.000010170 0.000079096 0.000048222

3 8 0.000093209 -0.000102061 0.000083801

4 8 -0.000058501 0.000076071 -0.000096419

5 6 0.000053779 -0.000031299 -0.000037985

6 16 -0.000014490 -0.000003816 0.000032180

7 6 -0.000008246 -0.000026783 0.000099526

8 16 -0.000004947 -0.000013568 -0.000065104

9 16 0.000053669 0.000026372 0.000033957

10 6 -0.000050067 0.000031312 -0.000010055

11 6 0.000017828 0.000013512 0.000004848

12 6 -0.000005249 -0.000000865 0.000008369

13 6 -0.000013213 0.000012273 -0.000013417

14 1 0.000014926 -0.000061922 0.000047374

15 1 0.000022080 0.000012361 -0.000013237

16 1 -0.000017397 -0.000056685 -0.000005594

17 1 0.000004274 -0.000047081 -0.000014701

18 1 -0.000013798 -0.000019117 -0.000019721

19 1 -0.000007051 0.000014583 0.000043157

20 1 0.000036649 -0.000010919 0.000021314

21 1 0.000001736 -0.000011195 -0.000032471

22 1 -0.000009515 0.000048409 -0.000007290

23 1 -0.000006865 0.000008427 0.000037234

24 1 -0.000001477 -0.000014634 0.000007776

25 1 -0.000001379 -0.000011693 -0.000015383

26 1 0.000008443 0.000000524 -0.000044551

27 1 0.000007009 0.000026373 -0.000033293

-------------------------------------------------------------------

Cartesian Forces: Max 0.000102061 RMS 0.000039744

Leave Link 716 at Sat Aug 17 17:49:13 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000166967 RMS 0.000030560

Search for a local minimum.

Step number 41 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .30560D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41

DE= -3.25D-06 DEPred=-1.22D-06 R= 2.66D+00

TightC=F SS= 1.41D+00 RLast= 1.88D-02 DXNew= 1.4142D-01 5.6502D-02

Trust test= 2.66D+00 RLast= 1.88D-02 DXMaxT set to 8.41D-02

ITU= 1 1 -1 -1 0 -1 -1 -1 0 -1 0 0 -1 -1 0 0 -1 0 0 -1

ITU= 1 -1 1 -1 1 1 -1 1 -1 1 1 -1 0 0 -1 0 0 -1 -1 0

ITU= 0

Eigenvalues --- 0.00075 0.00279 0.00289 0.00329 0.00374

Eigenvalues --- 0.00407 0.00674 0.01336 0.01840 0.02253

Eigenvalues --- 0.03477 0.03577 0.03749 0.04181 0.04375

Eigenvalues --- 0.04756 0.04804 0.04882 0.05327 0.05458

Eigenvalues --- 0.05485 0.05591 0.05682 0.05907 0.08208

Eigenvalues --- 0.08339 0.08672 0.11017 0.11986 0.12164

Eigenvalues --- 0.13659 0.14542 0.15633 0.15914 0.16033

Eigenvalues --- 0.16038 0.16102 0.16249 0.16936 0.18021

Eigenvalues --- 0.20078 0.21003 0.21904 0.22350 0.23247

Eigenvalues --- 0.24442 0.25108 0.25412 0.25896 0.27169

Eigenvalues --- 0.28139 0.28288 0.29174 0.29540 0.29709

Eigenvalues --- 0.30425 0.32463 0.32886 0.33571 0.33881

Eigenvalues --- 0.33918 0.33943 0.33970 0.34022 0.34079

Eigenvalues --- 0.34113 0.34222 0.34269 0.34704 0.34791

Eigenvalues --- 0.34945 0.35870 0.52495 0.56664 0.88787

En-DIIS/RFO-DIIS IScMMF= 0 using points: 41 40 39 38 37

RFO step: Lambda=-2.80133908D-07.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= -1.82D-05 SmlDif= 1.00D-05

RMS Error= 0.9812230575D-04 NUsed= 5 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.62206 0.38440 0.03166 -0.05774 0.01962

Iteration 1 RMS(Cart)= 0.00309562 RMS(Int)= 0.00000331

Iteration 2 RMS(Cart)= 0.00000525 RMS(Int)= 0.00000021

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000021

ITry= 1 IFail=0 DXMaxC= 9.34D-03 DCOld= 1.00D+10 DXMaxT= 8.41D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83533 0.00005 0.00025 -0.00007 0.00018 2.83552

R2 2.28965 -0.00017 -0.00028 0.00015 -0.00013 2.28951

R3 2.55324 -0.00005 0.00001 0.00001 0.00002 2.55325

R4 2.86502 -0.00001 -0.00004 -0.00012 -0.00016 2.86486

R5 3.61133 -0.00002 -0.00023 0.00053 0.00031 3.61164

R6 2.05840 -0.00004 -0.00002 -0.00010 -0.00012 2.05828

R7 1.83704 -0.00003 -0.00004 -0.00001 -0.00005 1.83699

R8 2.06131 -0.00002 0.00003 -0.00011 -0.00008 2.06123

R9 2.06858 -0.00001 -0.00002 0.00002 0.00000 2.06858

R10 2.06012 -0.00001 0.00002 -0.00005 -0.00003 2.06010

R11 3.31483 0.00003 -0.00013 0.00002 -0.00011 3.31472

R12 3.38753 -0.00003 -0.00002 -0.00004 -0.00006 3.38746

R13 3.25386 0.00002 -0.00014 0.00024 0.00010 3.25396

R14 3.47263 0.00000 0.00018 -0.00025 -0.00007 3.47255

R15 2.88128 -0.00001 -0.00005 0.00006 0.00002 2.88130

R16 2.06428 -0.00002 -0.00005 0.00003 -0.00002 2.06426

R17 2.06011 0.00000 0.00000 0.00000 0.00000 2.06011

R18 2.89426 -0.00002 -0.00007 0.00004 -0.00003 2.89422

R19 2.07223 -0.00001 -0.00005 0.00005 0.00000 2.07223

R20 2.07122 -0.00003 -0.00003 0.00000 -0.00004 2.07118

R21 2.88620 0.00000 0.00003 0.00001 0.00004 2.88624

R22 2.07202 -0.00002 -0.00007 0.00004 -0.00003 2.07198

R23 2.07182 -0.00001 -0.00001 -0.00001 -0.00002 2.07180

R24 2.06768 -0.00001 -0.00002 0.00001 -0.00001 2.06767

R25 2.06927 -0.00001 -0.00008 0.00007 -0.00002 2.06926

R26 2.06908 0.00000 0.00000 0.00000 0.00000 2.06907

A1 2.17596 0.00002 0.00022 -0.00021 0.00000 2.17596

A2 1.97751 0.00005 -0.00016 0.00023 0.00008 1.97758

A3 2.12912 -0.00007 -0.00007 -0.00003 -0.00011 2.12902

A4 2.02809 0.00003 0.00012 -0.00006 0.00006 2.02816

A5 1.82699 -0.00002 -0.00001 -0.00056 -0.00057 1.82642

A6 1.87403 0.00000 0.00009 0.00010 0.00019 1.87421

A7 1.94772 -0.00002 -0.00020 -0.00002 -0.00022 1.94750

A8 1.94142 -0.00001 0.00010 -0.00004 0.00006 1.94148

A9 1.83188 0.00002 -0.00013 0.00063 0.00050 1.83238

A10 1.87191 0.00003 0.00006 0.00024 0.00030 1.87221

A11 1.91306 0.00001 0.00019 -0.00019 0.00000 1.91306

A12 1.92631 -0.00001 0.00015 -0.00026 -0.00011 1.92619

A13 1.95259 0.00001 -0.00017 0.00033 0.00016 1.95275

A14 1.88347 0.00000 0.00003 -0.00006 -0.00003 1.88344

A15 1.89433 0.00000 -0.00013 0.00017 0.00003 1.89436

A16 1.89248 -0.00001 -0.00007 0.00001 -0.00006 1.89242

A17 1.79948 0.00012 -0.00002 0.00046 0.00044 1.79992

A18 1.97052 0.00002 0.00012 0.00003 0.00015 1.97067

A19 2.14237 0.00004 0.00012 0.00027 0.00039 2.14276

A20 2.15480 -0.00005 0.00006 -0.00007 -0.00001 2.15480

A21 1.79527 -0.00011 -0.00009 0.00010 0.00001 1.79528

A22 1.92702 -0.00002 0.00010 -0.00035 -0.00025 1.92678

A23 1.87866 -0.00001 0.00017 -0.00017 0.00000 1.87866

A24 1.89202 0.00004 -0.00003 0.00028 0.00025 1.89227

A25 1.93884 0.00003 0.00004 0.00006 0.00010 1.93894

A26 1.93858 -0.00004 -0.00020 0.00009 -0.00012 1.93847

A27 1.88680 0.00000 -0.00007 0.00010 0.00003 1.88683

A28 1.95260 0.00002 0.00006 0.00017 0.00023 1.95283

A29 1.91633 -0.00001 -0.00002 -0.00005 -0.00007 1.91626

A30 1.91707 -0.00001 0.00007 -0.00021 -0.00014 1.91693

A31 1.90694 -0.00001 -0.00012 0.00021 0.00009 1.90703

A32 1.90865 0.00000 0.00003 -0.00012 -0.00009 1.90856

A33 1.85990 0.00001 -0.00002 -0.00001 -0.00003 1.85988

A34 1.96622 0.00000 -0.00003 -0.00006 -0.00009 1.96613

A35 1.90629 -0.00001 0.00004 -0.00012 -0.00009 1.90621

A36 1.90766 0.00000 -0.00002 0.00017 0.00015 1.90781

A37 1.91273 0.00000 -0.00011 0.00008 -0.00003 1.91271

A38 1.91282 0.00000 0.00018 -0.00011 0.00007 1.91290

A39 1.85476 0.00000 -0.00007 0.00005 -0.00002 1.85474

A40 1.94535 0.00002 0.00007 0.00005 0.00012 1.94547

A41 1.94222 0.00000 0.00000 0.00005 0.00005 1.94227

A42 1.94278 0.00001 -0.00009 0.00007 -0.00002 1.94276

A43 1.87703 -0.00001 0.00002 -0.00010 -0.00008 1.87695

A44 1.87718 -0.00001 -0.00012 0.00004 -0.00008 1.87710

A45 1.87590 0.00000 0.00013 -0.00012 0.00000 1.87590

D1 2.73478 0.00002 0.00038 0.00166 0.00205 2.73683

D2 -1.39170 -0.00001 0.00020 0.00117 0.00137 -1.39033

D3 0.54902 0.00001 0.00008 0.00168 0.00176 0.55078

D4 -0.44334 0.00000 -0.00009 0.00125 0.00116 -0.44218

D5 1.71336 -0.00002 -0.00028 0.00076 0.00048 1.71384

D6 -2.62910 -0.00001 -0.00039 0.00126 0.00087 -2.62823

D7 -3.10050 0.00000 0.00056 -0.00037 0.00019 -3.10031

D8 0.00567 -0.00001 0.00011 -0.00078 -0.00067 0.00500

D9 3.13679 -0.00002 -0.00061 -0.00097 -0.00158 3.13520

D10 -1.07426 -0.00002 -0.00037 -0.00132 -0.00168 -1.07594

D11 1.03461 -0.00002 -0.00047 -0.00126 -0.00173 1.03289

D12 1.04408 0.00001 -0.00053 -0.00016 -0.00069 1.04339

D13 3.11623 0.00001 -0.00028 -0.00051 -0.00079 3.11543

D14 -1.05809 0.00000 -0.00038 -0.00045 -0.00084 -1.05892

D15 -0.99533 0.00000 -0.00031 -0.00091 -0.00122 -0.99655

D16 1.07681 0.00000 -0.00006 -0.00126 -0.00132 1.07549

D17 -3.09750 -0.00001 -0.00016 -0.00121 -0.00137 -3.09887

D18 -3.07738 -0.00003 0.00024 0.00122 0.00146 -3.07593

D19 -0.86986 -0.00003 0.00026 0.00075 0.00101 -0.86885

D20 1.23492 -0.00004 0.00019 0.00109 0.00128 1.23620

D21 1.82670 0.00001 0.00022 -0.00080 -0.00058 1.82612

D22 -1.13244 -0.00010 -0.00157 -0.00214 -0.00371 -1.13615

D23 2.58692 -0.00005 -0.00161 0.00169 0.00008 2.58700

D24 -0.73863 0.00007 0.00020 0.00308 0.00328 -0.73535

D25 -3.01861 -0.00004 -0.00265 -0.00219 -0.00484 -3.02345

D26 -0.89961 -0.00002 -0.00243 -0.00244 -0.00487 -0.90448

D27 1.13738 -0.00001 -0.00244 -0.00227 -0.00470 1.13268

D28 -3.12410 -0.00001 -0.00010 -0.00106 -0.00116 -3.12526

D29 -1.00375 0.00000 -0.00023 -0.00071 -0.00094 -1.00469

D30 1.03606 -0.00001 -0.00022 -0.00088 -0.00110 1.03496

D31 1.07619 0.00000 -0.00041 -0.00066 -0.00107 1.07512

D32 -3.08666 0.00000 -0.00053 -0.00031 -0.00085 -3.08750

D33 -1.04684 -0.00001 -0.00053 -0.00048 -0.00101 -1.04785

D34 -1.02461 0.00000 -0.00021 -0.00088 -0.00109 -1.02570

D35 1.09573 0.00001 -0.00033 -0.00054 -0.00087 1.09486

D36 3.13554 0.00000 -0.00033 -0.00070 -0.00103 3.13451

D37 -3.13067 0.00000 0.00087 -0.00099 -0.00012 -3.13079

D38 -1.00087 0.00000 0.00074 -0.00102 -0.00027 -1.00114

D39 1.02162 0.00000 0.00067 -0.00094 -0.00026 1.02136

D40 1.02676 0.00000 0.00094 -0.00118 -0.00024 1.02652

D41 -3.12662 0.00000 0.00081 -0.00121 -0.00040 -3.12702

D42 -1.10413 -0.00001 0.00074 -0.00113 -0.00039 -1.10452

D43 -1.00281 0.00000 0.00102 -0.00123 -0.00021 -1.00302

D44 1.12700 0.00000 0.00089 -0.00125 -0.00037 1.12663

D45 -3.13370 -0.00001 0.00082 -0.00117 -0.00036 -3.13405

D46 3.13948 -0.00001 0.00133 -0.00187 -0.00054 3.13894

D47 -1.04845 -0.00001 0.00140 -0.00193 -0.00053 -1.04897

D48 1.04364 -0.00001 0.00150 -0.00201 -0.00050 1.04314

D49 1.01331 0.00000 0.00137 -0.00172 -0.00035 1.01297

D50 3.10857 0.00000 0.00145 -0.00178 -0.00034 3.10824

D51 -1.08252 0.00000 0.00155 -0.00186 -0.00031 -1.08283

D52 -1.01573 0.00000 0.00141 -0.00176 -0.00035 -1.01608

D53 1.07953 0.00000 0.00149 -0.00183 -0.00034 1.07919

D54 -3.11157 0.00000 0.00159 -0.00190 -0.00031 -3.11188

Item Value Threshold Converged?

Maximum Force 0.000167 0.000450 YES

RMS Force 0.000031 0.000300 YES

Maximum Displacement 0.009340 0.001800 NO

RMS Displacement 0.003096 0.001200 NO

Predicted change in Energy=-6.002634D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:49:13 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.089048 -0.414940 -0.219505

2 6 0 -2.849272 0.077954 0.467142

3 8 0 -4.871488 0.289712 -0.818776

4 8 0 -4.241549 -1.755629 -0.149980

5 6 0 -2.308112 -0.796760 1.580847

6 16 0 -1.572845 0.296539 -0.938426

7 6 0 -0.114554 0.764080 -0.083110

8 16 0 1.083818 -0.564157 0.030881

9 16 0 0.020882 2.242452 0.789291

10 6 0 2.688986 0.330107 0.008762

11 6 0 3.847061 -0.658604 -0.069214

12 6 0 5.204502 0.050629 -0.066455

13 6 0 6.377255 -0.923417 -0.159296

14 1 0 -3.053203 1.087351 0.821927

15 1 0 -5.043794 -1.981161 -0.650483

16 1 0 -1.408055 -0.343280 1.997987

17 1 0 -3.044012 -0.886807 2.386196

18 1 0 -2.059989 -1.797686 1.227263

19 1 0 2.683734 0.998349 -0.855341

20 1 0 2.755331 0.941090 0.909179

21 1 0 3.800028 -1.353161 0.778053

22 1 0 3.756648 -1.266341 -0.976817

23 1 0 5.244987 0.755755 -0.905117

24 1 0 5.297360 0.652226 0.845378

25 1 0 7.336295 -0.396690 -0.158517

26 1 0 6.382854 -1.620420 0.685210

27 1 0 6.328339 -1.518828 -1.076855

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.500491 0.000000

3 O 1.211558 2.405781 0.000000

4 O 1.351124 2.383548 2.242216 0.000000

5 C 2.561013 1.516020 3.675529 2.766473 0.000000

6 S 2.711887 1.911195 3.300819 3.457604 2.843001

7 C 4.147927 2.872669 4.836801 4.835855 3.164912

8 S 5.181072 4.008968 6.075909 5.460023 3.736534

9 S 4.997092 3.609240 5.507663 5.919054 3.909934

10 C 6.822679 5.562912 7.605736 7.239324 5.358382

11 C 7.941271 6.758037 8.801945 8.163063 6.374004

12 C 9.306463 8.071477 10.106864 9.617558 7.737637

13 C 10.478821 9.301826 11.333173 10.651369 8.858879

14 H 2.101056 1.089194 2.575712 3.230991 2.163561

15 H 1.884231 3.210135 2.283610 0.972093 3.723654

16 H 3.479961 2.144301 4.508902 3.825856 1.090757

17 H 2.846829 2.156723 3.872429 2.936176 1.094644

18 H 2.849948 2.172274 4.055617 2.580266 1.090156

19 H 6.947824 5.762833 7.588470 7.486086 5.837462

20 H 7.068116 5.687879 7.847196 7.573007 5.395341

21 H 8.007054 6.808667 8.969063 8.104949 6.185744

22 H 7.928011 6.894224 8.768752 8.055695 6.598747

23 H 9.432115 8.237690 10.127571 9.842339 8.101828

24 H 9.506707 8.175602 10.310494 9.888341 7.777125

25 H 11.425521 10.215797 12.244879 11.657327 9.808161

26 H 10.579813 9.389579 11.513939 10.658038 8.775732

27 H 10.510736 9.442573 11.347843 10.613092 9.064935

6 7 8 9 10

6 S 0.000000

7 C 1.754073 0.000000

8 S 2.956046 1.792569 0.000000

9 S 3.051483 1.721920 3.095493 0.000000

10 C 4.365947 2.838417 1.837597 3.374177 0.000000

11 C 5.571642 4.209348 2.766668 4.877786 1.524718

12 C 6.837633 5.366716 4.167430 5.692653 2.532110

13 C 8.080806 6.707984 5.309022 7.164219 3.899089

14 H 2.432219 3.091804 4.524177 3.284102 5.848709

15 H 4.161528 5.670596 6.326119 6.750022 8.097681

16 H 3.009824 2.688932 3.182409 3.191993 4.603934

17 H 3.823317 4.171885 4.763464 4.662183 6.324582

18 H 3.051769 3.473390 3.582799 4.565584 5.344624

19 H 4.314847 2.912326 2.405524 3.367995 1.092360

20 H 4.749967 3.041744 2.414773 3.030698 1.090161

21 H 5.876698 4.533020 2.925507 5.216370 2.158614

22 H 5.554058 4.461786 2.941520 5.420952 2.158684

23 H 6.833360 5.422218 4.464704 5.689689 2.747634

24 H 7.106911 5.492123 4.460598 5.511188 2.758134

25 H 8.970039 7.541103 6.257587 7.834455 4.706772

26 H 8.342906 6.963654 5.442759 7.443609 4.231643

27 H 8.108232 6.907248 5.444583 7.577186 4.223981

11 12 13 14 15

11 C 0.000000

12 C 1.531556 0.000000

13 C 2.545609 1.527330 0.000000

14 H 7.173293 8.369809 9.692241 0.000000

15 H 9.007459 10.464073 11.480438 3.942868 0.000000

16 H 5.655881 6.938515 8.099475 2.477162 4.787028

17 H 7.319016 8.656342 9.759157 2.518794 3.797124

18 H 6.153990 7.606760 8.594997 3.078021 3.530253

19 H 2.171823 2.806204 4.221346 5.977759 8.284572

20 H 2.169826 2.782664 4.211456 5.811030 8.473396

21 H 1.096578 2.157862 2.775861 7.274944 8.980439

22 H 1.096021 2.158576 2.766500 7.426266 8.835453

23 H 2.157160 1.096446 2.158217 8.482488 10.649627

24 H 2.158268 1.096349 2.158285 8.361925 10.775518

25 H 3.500190 2.180164 1.094166 10.540651 12.490764

26 H 2.815048 2.178514 1.095004 9.817836 11.510104

27 H 2.812840 2.178788 1.094907 9.920226 11.389511

16 17 18 19 20

16 H 0.000000

17 H 1.767055 0.000000

18 H 1.770404 1.772323 0.000000

19 H 5.165675 6.846054 5.887101 0.000000

20 H 4.490979 6.257409 5.548817 1.766900 0.000000

21 H 5.443550 7.045885 5.893996 3.073059 2.524317

22 H 6.031224 7.596241 6.242881 2.508929 3.071216

23 H 7.341584 9.068531 8.026816 2.573197 3.086164

24 H 6.876201 8.620976 7.763922 3.137401 2.559185

25 H 9.006499 10.698905 9.600694 4.906936 4.890283

26 H 8.003296 9.607151 8.462083 4.786934 4.446395

27 H 8.407637 10.011650 8.703492 4.434906 4.770945

21 22 23 24 25

21 H 0.000000

22 H 1.757551 0.000000

23 H 3.060799 2.511805 0.000000

24 H 2.503620 3.061876 1.754336 0.000000

25 H 3.781162 3.773564 2.501822 2.503055 0.000000

26 H 2.598276 3.128045 3.077351 2.523663 1.765911

27 H 3.140141 2.585992 2.525247 3.077559 1.765931

26 27

26 H 0.000000

27 H 1.765833 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 6.92D-04

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.100314 -0.472049 -0.138096

2 6 0 -2.854412 0.129925 0.442276

3 8 0 -4.887112 0.119395 -0.844506

4 8 0 -4.253407 -1.779832 0.164893

5 6 0 -2.304737 -0.538916 1.686794

6 16 0 -1.589578 0.097649 -0.990142

7 6 0 -0.123784 0.703498 -0.241033

8 16 0 1.074330 -0.587420 0.092669

9 16 0 0.020234 2.310797 0.359682

10 6 0 2.680043 0.285629 -0.097681

11 6 0 3.836556 -0.704251 -0.011767

12 6 0 5.194596 -0.008507 -0.143423

13 6 0 6.365677 -0.986566 -0.074816

14 1 0 -3.054485 1.186127 0.617636

15 1 0 -5.060003 -2.087149 -0.282237

16 1 0 -1.400830 -0.021861 2.011380

17 1 0 -3.033964 -0.485754 2.501439

18 1 0 -2.060457 -1.586670 1.510785

19 1 0 2.668162 0.793336 -1.064813

20 1 0 2.754444 1.043807 0.682115

21 1 0 3.795992 -1.240680 0.943786

22 1 0 3.738032 -1.460428 -0.799010

23 1 0 5.228694 0.539841 -1.092289

24 1 0 5.295597 0.742353 0.649035

25 1 0 7.325152 -0.469964 -0.173448

26 1 0 6.377717 -1.526007 0.878019

27 1 0 6.308574 -1.732434 -0.874343

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2997926 0.1934826 0.1810437

Leave Link 202 at Sat Aug 17 17:49:13 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.3847966262 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0550027278 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.3297938984 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2319

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.29D-07

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 97

GePol: Fraction of low-weight points (<1% of avg) = 4.18%

GePol: Cavity surface area = 309.034 Ang\*\*2

GePol: Cavity volume = 320.311 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057667571 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.3240271413 Hartrees.

Leave Link 301 at Sat Aug 17 17:49:13 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:49:13 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:49:13 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000606 -0.000043 0.000066 Ang= -0.07 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 17:49:14 2019, MaxMem= 1342177280 cpu: 2.6

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16133283.

Iteration 1 A\*A^-1 deviation from unit magnitude is 4.44D-15 for 2282.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.80D-15 for 881 423.

Iteration 1 A^-1\*A deviation from unit magnitude is 3.77D-15 for 2290.

Iteration 1 A^-1\*A deviation from orthogonality is 2.56D-11 for 2127 891.

E= -1658.67697044317

DIIS: error= 2.06D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67697044317 IErMin= 1 ErrMin= 2.06D-04

ErrMax= 2.06D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.00D-05 BMatP= 4.00D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.06D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.428 Goal= None Shift= 0.000

Gap= 0.484 Goal= None Shift= 0.000

RMSDP=1.61D-05 MaxDP=4.04D-04 OVMax= 9.82D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.61D-05 CP: 1.00D+00

E= -1658.67698998096 Delta-E= -0.000019537795 Rises=F Damp=F

DIIS: error= 2.04D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67698998096 IErMin= 2 ErrMin= 2.04D-05

ErrMax= 2.04D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.57D-07 BMatP= 4.00D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.610D-01 0.106D+01

Coeff: -0.610D-01 0.106D+01

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.20D-06 MaxDP=1.51D-04 DE=-1.95D-05 OVMax= 2.37D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.98D-06 CP: 1.00D+00 1.07D+00

E= -1658.67699017159 Delta-E= -0.000000190624 Rises=F Damp=F

DIIS: error= 1.36D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67699017159 IErMin= 3 ErrMin= 1.36D-05

ErrMax= 1.36D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.91D-07 BMatP= 6.57D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.359D-01 0.489D+00 0.547D+00

Coeff: -0.359D-01 0.489D+00 0.547D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.81D-06 MaxDP=7.63D-05 DE=-1.91D-07 OVMax= 1.92D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.32D-06 CP: 1.00D+00 1.10D+00 6.23D-01

E= -1658.67699024245 Delta-E= -0.000000070859 Rises=F Damp=F

DIIS: error= 7.92D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67699024245 IErMin= 4 ErrMin= 7.92D-06

ErrMax= 7.92D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.35D-07 BMatP= 3.91D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.147D-01 0.176D+00 0.371D+00 0.468D+00

Coeff: -0.147D-01 0.176D+00 0.371D+00 0.468D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.93D-07 MaxDP=3.59D-05 DE=-7.09D-08 OVMax= 7.49D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.14D-07 CP: 1.00D+00 1.11D+00 7.00D-01 6.21D-01

E= -1658.67699027777 Delta-E= -0.000000035328 Rises=F Damp=F

DIIS: error= 1.29D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67699027777 IErMin= 5 ErrMin= 1.29D-06

ErrMax= 1.29D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.37D-09 BMatP= 1.35D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.180D-02 0.128D-01 0.937D-01 0.196D+00 0.699D+00

Coeff: -0.180D-02 0.128D-01 0.937D-01 0.196D+00 0.699D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.13D-07 MaxDP=1.13D-05 DE=-3.53D-08 OVMax= 2.39D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.30D-07 CP: 1.00D+00 1.11D+00 7.37D-01 7.13D-01 9.14D-01

E= -1658.67699027909 Delta-E= -0.000000001311 Rises=F Damp=F

DIIS: error= 5.45D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67699027909 IErMin= 6 ErrMin= 5.45D-07

ErrMax= 5.45D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.33D-10 BMatP= 4.37D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.936D-03-0.166D-01 0.316D-03 0.402D-01 0.347D+00 0.628D+00

Coeff: 0.936D-03-0.166D-01 0.316D-03 0.402D-01 0.347D+00 0.628D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=7.61D-08 MaxDP=3.22D-06 DE=-1.31D-09 OVMax= 1.12D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.80D-08 CP: 1.00D+00 1.11D+00 7.46D-01 7.35D-01 9.76D-01

CP: 9.14D-01

E= -1658.67699027931 Delta-E= -0.000000000223 Rises=F Damp=F

DIIS: error= 2.78D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67699027931 IErMin= 7 ErrMin= 2.78D-07

ErrMax= 2.78D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.10D-10 BMatP= 8.33D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.692D-03-0.912D-02-0.160D-01-0.171D-01 0.272D-01 0.274D+00

Coeff-Com: 0.740D+00

Coeff: 0.692D-03-0.912D-02-0.160D-01-0.171D-01 0.272D-01 0.274D+00

Coeff: 0.740D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.05D-08 MaxDP=1.95D-06 DE=-2.23D-10 OVMax= 6.99D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.92D-08 CP: 1.00D+00 1.11D+00 7.48D-01 7.49D-01 1.01D+00

CP: 1.08D+00 1.12D+00

E= -1658.67699027938 Delta-E= -0.000000000070 Rises=F Damp=F

DIIS: error= 1.30D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67699027938 IErMin= 8 ErrMin= 1.30D-07

ErrMax= 1.30D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.11D-11 BMatP= 1.10D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.165D-03-0.132D-02-0.750D-02-0.145D-01-0.437D-01 0.188D-01

Coeff-Com: 0.336D+00 0.712D+00

Coeff: 0.165D-03-0.132D-02-0.750D-02-0.145D-01-0.437D-01 0.188D-01

Coeff: 0.336D+00 0.712D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.75D-08 MaxDP=7.22D-07 DE=-7.05D-11 OVMax= 3.05D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 7.77D-09 CP: 1.00D+00 1.11D+00 7.50D-01 7.53D-01 1.02D+00

CP: 1.16D+00 1.25D+00 9.88D-01

E= -1658.67699027937 Delta-E= 0.000000000006 Rises=F Damp=F

DIIS: error= 4.51D-08 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 8 EnMin= -1658.67699027938 IErMin= 9 ErrMin= 4.51D-08

ErrMax= 4.51D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.78D-12 BMatP= 2.11D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.589D-04 0.123D-02-0.519D-03-0.328D-02-0.263D-01-0.468D-01

Coeff-Com: 0.665D-02 0.338D+00 0.731D+00

Coeff: -0.589D-04 0.123D-02-0.519D-03-0.328D-02-0.263D-01-0.468D-01

Coeff: 0.665D-02 0.338D+00 0.731D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=8.20D-09 MaxDP=4.35D-07 DE= 6.37D-12 OVMax= 1.33D-06

Error on total polarization charges = 0.04163

SCF Done: E(UB3LYP) = -1658.67699028 A.U. after 9 cycles

NFock= 9 Conv=0.82D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655235153845D+03 PE=-6.147416321468D+03 EE= 1.731180150202D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.62

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:49:34 2019, MaxMem= 1342177280 cpu: 235.5

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 337

Leave Link 701 at Sat Aug 17 17:49:35 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:49:35 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:49:38 2019, MaxMem= 1342177280 cpu: 38.5

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.39982443D+00-2.93214469D+00 6.56710621D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000001299 -0.000007954 -0.000079727

2 6 -0.000043182 -0.000023850 0.000000758

3 8 0.000002973 -0.000001874 0.000072291

4 8 -0.000018220 0.000050974 -0.000010827

5 6 0.000014588 -0.000032317 0.000011248

6 16 0.000030193 0.000034309 0.000031789

7 6 -0.000015124 0.000016059 0.000042484

8 16 -0.000008032 0.000005057 -0.000008543

9 16 -0.000002818 -0.000022500 0.000048974

10 6 -0.000007205 0.000007233 -0.000001098

11 6 0.000005330 0.000001193 -0.000011067

12 6 -0.000004919 -0.000001370 -0.000007106

13 6 -0.000006598 0.000008498 -0.000012413

14 1 0.000012893 -0.000014135 0.000039653

15 1 0.000011432 0.000040308 -0.000040014

16 1 0.000011866 -0.000044296 0.000011233

17 1 0.000005840 -0.000051601 -0.000008719

18 1 -0.000003016 -0.000011881 -0.000041417

19 1 0.000010445 0.000028252 0.000040313

20 1 -0.000000382 -0.000027453 0.000024226

21 1 0.000001969 -0.000006607 -0.000034969

22 1 0.000006441 0.000029062 -0.000022910

23 1 -0.000001026 0.000020112 0.000032126

24 1 -0.000002971 -0.000020554 0.000018488

25 1 -0.000002978 0.000000602 -0.000012172

26 1 -0.000001015 -0.000006524 -0.000044302

27 1 0.000002215 0.000031257 -0.000038302

-------------------------------------------------------------------

Cartesian Forces: Max 0.000079727 RMS 0.000025612

Leave Link 716 at Sat Aug 17 17:49:38 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000054315 RMS 0.000011092

Search for a local minimum.

Step number 42 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .11092D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

DE= -1.69D-06 DEPred=-6.00D-07 R= 2.82D+00

TightC=F SS= 1.41D+00 RLast= 1.18D-02 DXNew= 1.4142D-01 3.5432D-02

Trust test= 2.82D+00 RLast= 1.18D-02 DXMaxT set to 8.41D-02

ITU= 1 1 1 -1 -1 0 -1 -1 -1 0 -1 0 0 -1 -1 0 0 -1 0 0

ITU= -1 1 -1 1 -1 1 1 -1 1 -1 1 1 -1 0 0 -1 0 0 -1 -1

ITU= 0 0

Eigenvalues --- 0.00086 0.00268 0.00288 0.00332 0.00370

Eigenvalues --- 0.00399 0.00645 0.01253 0.01852 0.02294

Eigenvalues --- 0.03470 0.03574 0.03869 0.04284 0.04764

Eigenvalues --- 0.04803 0.04870 0.05163 0.05287 0.05459

Eigenvalues --- 0.05483 0.05583 0.05662 0.05942 0.08245

Eigenvalues --- 0.08342 0.08717 0.11007 0.11994 0.12164

Eigenvalues --- 0.13714 0.14543 0.15673 0.15970 0.16022

Eigenvalues --- 0.16058 0.16134 0.16327 0.17374 0.18061

Eigenvalues --- 0.20000 0.21372 0.21949 0.22438 0.23176

Eigenvalues --- 0.24431 0.25092 0.25596 0.25810 0.27170

Eigenvalues --- 0.28183 0.28580 0.29150 0.29531 0.29714

Eigenvalues --- 0.30716 0.32492 0.33362 0.33532 0.33881

Eigenvalues --- 0.33924 0.33946 0.33975 0.34022 0.34060

Eigenvalues --- 0.34106 0.34215 0.34294 0.34696 0.34909

Eigenvalues --- 0.35468 0.35575 0.52476 0.56385 0.88925

En-DIIS/RFO-DIIS IScMMF= 0 using points: 42 41 40 39 38

RFO step: Lambda=-3.36592134D-08.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= -3.48D-06 SmlDif= 1.00D-05

RMS Error= 0.3617571196D-04 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 0.86960 0.03406 0.07136 0.01058 0.01439

Iteration 1 RMS(Cart)= 0.00173668 RMS(Int)= 0.00000125

Iteration 2 RMS(Cart)= 0.00000183 RMS(Int)= 0.00000009

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000009

ITry= 1 IFail=0 DXMaxC= 9.17D-03 DCOld= 1.00D+10 DXMaxT= 8.41D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83552 0.00000 -0.00001 -0.00001 -0.00002 2.83550

R2 2.28951 -0.00005 -0.00004 0.00001 -0.00004 2.28947

R3 2.55325 -0.00005 -0.00002 -0.00009 -0.00010 2.55315

R4 2.86486 0.00002 0.00004 0.00005 0.00009 2.86495

R5 3.61164 0.00000 -0.00010 -0.00008 -0.00018 3.61146

R6 2.05828 0.00000 0.00001 -0.00003 -0.00002 2.05826

R7 1.83699 -0.00001 -0.00001 -0.00001 -0.00002 1.83697

R8 2.06123 0.00001 0.00001 0.00002 0.00003 2.06126

R9 2.06858 0.00000 -0.00001 0.00002 0.00001 2.06858

R10 2.06010 -0.00001 0.00000 -0.00003 -0.00003 2.06006

R11 3.31472 -0.00003 0.00001 0.00002 0.00002 3.31474

R12 3.38746 0.00000 0.00002 0.00000 0.00002 3.38748

R13 3.25396 -0.00002 -0.00008 0.00003 -0.00005 3.25391

R14 3.47255 0.00000 0.00002 -0.00006 -0.00004 3.47252

R15 2.88130 0.00000 -0.00002 0.00003 0.00001 2.88131

R16 2.06426 -0.00001 -0.00001 -0.00001 -0.00002 2.06424

R17 2.06011 -0.00001 -0.00001 -0.00003 -0.00003 2.06007

R18 2.89422 -0.00002 -0.00002 -0.00003 -0.00005 2.89417

R19 2.07223 -0.00001 -0.00002 -0.00001 -0.00003 2.07220

R20 2.07118 -0.00001 0.00000 -0.00001 -0.00002 2.07116

R21 2.88624 -0.00001 0.00000 -0.00003 -0.00003 2.88621

R22 2.07198 -0.00001 -0.00002 -0.00002 -0.00004 2.07195

R23 2.07180 0.00000 0.00000 0.00000 0.00000 2.07179

R24 2.06767 0.00000 -0.00001 0.00000 -0.00002 2.06766

R25 2.06926 -0.00001 -0.00002 -0.00001 -0.00003 2.06923

R26 2.06907 0.00000 0.00000 0.00000 0.00000 2.06907

A1 2.17596 0.00001 0.00008 0.00000 0.00008 2.17604

A2 1.97758 0.00001 -0.00006 0.00008 0.00002 1.97761

A3 2.12902 -0.00002 -0.00001 -0.00007 -0.00009 2.12893

A4 2.02816 0.00002 -0.00002 0.00004 0.00001 2.02817

A5 1.82642 0.00001 0.00017 0.00022 0.00040 1.82682

A6 1.87421 0.00000 0.00002 0.00000 0.00003 1.87424

A7 1.94750 -0.00002 -0.00003 -0.00007 -0.00010 1.94740

A8 1.94148 -0.00001 -0.00001 -0.00012 -0.00013 1.94135

A9 1.83238 0.00000 -0.00013 -0.00007 -0.00020 1.83218

A10 1.87221 -0.00003 -0.00005 -0.00007 -0.00012 1.87209

A11 1.91306 0.00001 0.00004 -0.00003 0.00001 1.91307

A12 1.92619 0.00001 0.00006 0.00000 0.00006 1.92626

A13 1.95275 -0.00002 -0.00008 -0.00002 -0.00010 1.95265

A14 1.88344 -0.00001 0.00003 -0.00005 -0.00002 1.88342

A15 1.89436 0.00000 -0.00004 0.00003 -0.00001 1.89435

A16 1.89242 0.00001 0.00000 0.00006 0.00006 1.89248

A17 1.79992 -0.00002 -0.00010 -0.00011 -0.00021 1.79971

A18 1.97067 -0.00002 -0.00004 -0.00021 -0.00025 1.97042

A19 2.14276 0.00000 -0.00002 0.00005 0.00002 2.14278

A20 2.15480 0.00002 0.00009 0.00008 0.00017 2.15497

A21 1.79528 0.00001 0.00003 0.00005 0.00008 1.79536

A22 1.92678 0.00001 0.00002 -0.00001 0.00001 1.92679

A23 1.87866 0.00001 0.00009 0.00006 0.00015 1.87881

A24 1.89227 -0.00001 -0.00008 0.00001 -0.00007 1.89220

A25 1.93894 0.00000 0.00001 0.00000 0.00001 1.93895

A26 1.93847 -0.00001 -0.00002 -0.00005 -0.00007 1.93840

A27 1.88683 0.00000 -0.00002 -0.00001 -0.00003 1.88680

A28 1.95283 -0.00001 0.00000 -0.00005 -0.00005 1.95278

A29 1.91626 0.00000 -0.00001 0.00001 0.00000 1.91626

A30 1.91693 0.00001 0.00005 0.00002 0.00006 1.91699

A31 1.90703 0.00000 -0.00002 -0.00002 -0.00004 1.90699

A32 1.90856 0.00000 0.00000 0.00001 0.00000 1.90857

A33 1.85988 0.00000 -0.00001 0.00003 0.00003 1.85990

A34 1.96613 0.00000 0.00000 0.00003 0.00003 1.96616

A35 1.90621 0.00000 0.00002 -0.00002 0.00000 1.90621

A36 1.90781 -0.00001 -0.00002 -0.00002 -0.00004 1.90777

A37 1.91271 0.00000 -0.00001 0.00003 0.00002 1.91273

A38 1.91290 0.00000 0.00002 -0.00004 -0.00002 1.91288

A39 1.85474 0.00000 -0.00001 0.00001 0.00000 1.85474

A40 1.94547 0.00000 0.00000 0.00000 0.00000 1.94547

A41 1.94227 0.00000 -0.00001 -0.00002 -0.00004 1.94223

A42 1.94276 0.00000 -0.00002 0.00006 0.00004 1.94280

A43 1.87695 0.00000 0.00002 -0.00003 -0.00001 1.87694

A44 1.87710 0.00000 -0.00001 -0.00001 -0.00002 1.87709

A45 1.87590 0.00000 0.00002 -0.00001 0.00002 1.87592

D1 2.73683 -0.00001 -0.00056 -0.00216 -0.00272 2.73411

D2 -1.39033 -0.00002 -0.00048 -0.00205 -0.00253 -1.39287

D3 0.55078 -0.00002 -0.00054 -0.00203 -0.00258 0.54820

D4 -0.44218 0.00001 -0.00027 -0.00199 -0.00226 -0.44444

D5 1.71384 0.00001 -0.00020 -0.00188 -0.00208 1.71177

D6 -2.62823 0.00001 -0.00026 -0.00186 -0.00212 -2.63035

D7 -3.10031 0.00000 -0.00005 0.00009 0.00004 -3.10028

D8 0.00500 0.00002 0.00023 0.00026 0.00048 0.00549

D9 3.13520 0.00000 0.00042 0.00017 0.00059 3.13580

D10 -1.07594 0.00000 0.00052 0.00009 0.00061 -1.07533

D11 1.03289 0.00000 0.00050 0.00016 0.00066 1.03355

D12 1.04339 -0.00001 0.00023 -0.00011 0.00013 1.04352

D13 3.11543 -0.00001 0.00033 -0.00018 0.00015 3.11558

D14 -1.05892 -0.00001 0.00031 -0.00012 0.00020 -1.05873

D15 -0.99655 0.00000 0.00042 0.00010 0.00053 -0.99602

D16 1.07549 0.00001 0.00052 0.00003 0.00055 1.07604

D17 -3.09887 0.00001 0.00050 0.00009 0.00060 -3.09827

D18 -3.07593 -0.00001 -0.00023 -0.00142 -0.00165 -3.07758

D19 -0.86885 0.00001 -0.00016 -0.00126 -0.00142 -0.87027

D20 1.23620 -0.00001 -0.00027 -0.00148 -0.00176 1.23444

D21 1.82612 0.00000 0.00008 -0.00017 -0.00009 1.82602

D22 -1.13615 0.00000 -0.00004 0.00028 0.00024 -1.13591

D23 2.58700 0.00001 -0.00051 0.00172 0.00121 2.58821

D24 -0.73535 0.00001 -0.00040 0.00127 0.00086 -0.73449

D25 -3.02345 -0.00001 -0.00017 -0.00004 -0.00021 -3.02366

D26 -0.90448 0.00000 -0.00010 0.00000 -0.00010 -0.90458

D27 1.13268 0.00000 -0.00011 0.00002 -0.00009 1.13259

D28 -3.12526 0.00001 0.00000 0.00038 0.00038 -3.12487

D29 -1.00469 0.00001 -0.00003 0.00033 0.00030 -1.00440

D30 1.03496 0.00001 -0.00002 0.00039 0.00037 1.03533

D31 1.07512 0.00000 -0.00013 0.00031 0.00018 1.07530

D32 -3.08750 -0.00001 -0.00016 0.00026 0.00010 -3.08741

D33 -1.04785 0.00000 -0.00015 0.00032 0.00017 -1.04768

D34 -1.02570 0.00000 -0.00009 0.00035 0.00026 -1.02544

D35 1.09486 0.00000 -0.00013 0.00031 0.00018 1.09503

D36 3.13451 0.00000 -0.00012 0.00036 0.00025 3.13476

D37 -3.13079 0.00000 0.00001 -0.00022 -0.00021 -3.13100

D38 -1.00114 0.00000 0.00001 -0.00017 -0.00016 -1.00130

D39 1.02136 0.00000 0.00000 -0.00018 -0.00018 1.02118

D40 1.02652 0.00000 0.00004 -0.00019 -0.00015 1.02637

D41 -3.12702 0.00000 0.00004 -0.00014 -0.00010 -3.12711

D42 -1.10452 0.00000 0.00003 -0.00015 -0.00012 -1.10463

D43 -1.00302 0.00000 0.00006 -0.00022 -0.00016 -1.00318

D44 1.12663 0.00000 0.00007 -0.00018 -0.00011 1.12652

D45 -3.13405 0.00000 0.00005 -0.00018 -0.00013 -3.13418

D46 3.13894 0.00000 0.00014 -0.00037 -0.00023 3.13871

D47 -1.04897 0.00000 0.00015 -0.00042 -0.00027 -1.04924

D48 1.04314 0.00000 0.00016 -0.00040 -0.00024 1.04290

D49 1.01297 0.00000 0.00012 -0.00039 -0.00027 1.01270

D50 3.10824 0.00000 0.00013 -0.00044 -0.00031 3.10793

D51 -1.08283 0.00000 0.00014 -0.00042 -0.00028 -1.08311

D52 -1.01608 0.00000 0.00012 -0.00040 -0.00028 -1.01636

D53 1.07919 0.00000 0.00014 -0.00045 -0.00031 1.07888

D54 -3.11188 0.00000 0.00015 -0.00043 -0.00028 -3.11217

Item Value Threshold Converged?

Maximum Force 0.000054 0.000450 YES

RMS Force 0.000011 0.000300 YES

Maximum Displacement 0.009168 0.001800 NO

RMS Displacement 0.001737 0.001200 NO

Predicted change in Energy=-8.148637D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:49:38 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.089810 -0.414150 -0.217881

2 6 0 -2.848681 0.077433 0.467237

3 8 0 -4.873685 0.291607 -0.813925

4 8 0 -4.242230 -1.754905 -0.150570

5 6 0 -2.307050 -0.797858 1.580325

6 16 0 -1.573394 0.295203 -0.939364

7 6 0 -0.114794 0.763863 -0.085165

8 16 0 1.083710 -0.564239 0.029151

9 16 0 0.020560 2.242770 0.786288

10 6 0 2.688828 0.330086 0.007621

11 6 0 3.847000 -0.658570 -0.069718

12 6 0 5.204351 0.050773 -0.065909

13 6 0 6.377284 -0.923125 -0.157803

14 1 0 -3.051131 1.086984 0.822398

15 1 0 -5.045456 -1.979355 -0.649965

16 1 0 -1.406332 -0.345015 1.996766

17 1 0 -3.042256 -0.887665 2.386338

18 1 0 -2.059829 -1.798803 1.226216

19 1 0 2.684029 0.998347 -0.856458

20 1 0 2.754736 0.941059 0.908056

21 1 0 3.799462 -1.353204 0.777439

22 1 0 3.757285 -1.266203 -0.977449

23 1 0 5.245412 0.755909 -0.904509

24 1 0 5.296410 0.652360 0.846009

25 1 0 7.336246 -0.396274 -0.156516

26 1 0 6.382423 -1.619910 0.686868

27 1 0 6.329072 -1.518754 -1.075256

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.500480 0.000000

3 O 1.211537 2.405803 0.000000

4 O 1.351068 2.383511 2.242094 0.000000

5 C 2.561056 1.516068 3.675184 2.767103 0.000000

6 S 2.712207 1.911101 3.302676 3.456562 2.842862

7 C 4.148021 2.872364 4.837475 4.835721 3.165251

8 S 5.181588 4.008411 6.077319 5.460368 3.736037

9 S 4.996270 3.608743 5.506483 5.918656 3.910713

10 C 6.823098 5.562292 7.607104 7.239598 5.357654

11 C 7.941955 6.757379 8.803808 8.163586 6.372941

12 C 9.307023 8.070705 10.108627 9.617980 7.736369

13 C 10.479634 9.301088 11.335360 10.652042 8.857452

14 H 2.101056 1.089183 2.575244 3.231365 2.163501

15 H 1.884097 3.210037 2.283343 0.972083 3.724110

16 H 3.480013 2.144363 4.508637 3.826377 1.090772

17 H 2.846672 2.156811 3.871240 2.937337 1.094646

18 H 2.850175 2.172233 4.055832 2.580763 1.090139

19 H 6.948943 5.762910 7.590806 7.486770 5.837390

20 H 7.067682 5.686691 7.847281 7.572744 5.394206

21 H 8.007065 6.807405 8.970024 8.105022 6.184054

22 H 7.929680 6.894292 8.771953 8.056972 6.598311

23 H 9.433285 8.237498 10.130149 9.843169 8.101128

24 H 9.506336 8.174137 10.310982 9.888061 7.775278

25 H 11.426234 10.214999 12.246950 11.657916 9.806683

26 H 10.580174 9.388424 11.515479 10.658461 8.773881

27 H 10.512295 9.442365 11.351100 10.614294 9.063907

6 7 8 9 10

6 S 0.000000

7 C 1.754085 0.000000

8 S 2.955819 1.792577 0.000000

9 S 3.051489 1.721893 3.095616 0.000000

10 C 4.366296 2.838498 1.837576 3.374068 0.000000

11 C 5.571952 4.209438 2.766667 4.877721 1.524725

12 C 6.838165 5.366766 4.167369 5.692344 2.532050

13 C 8.081365 6.708076 5.309019 7.163947 3.899053

14 H 2.431960 3.090332 4.522464 3.282138 5.846698

15 H 4.160838 5.670597 6.326960 6.749346 8.098462

16 H 3.009759 2.689259 3.181175 3.193417 4.602477

17 H 3.823222 4.172038 4.762828 4.662684 6.323491

18 H 3.051428 3.474210 3.583148 4.566822 5.344800

19 H 4.315894 2.912608 2.405618 3.367679 1.092350

20 H 4.750032 3.041725 2.414689 3.030676 1.090144

21 H 5.876415 4.532931 2.925357 5.216436 2.158609

22 H 5.554780 4.462100 2.941768 5.420956 2.158727

23 H 6.834442 5.422472 4.464782 5.689343 2.747623

24 H 7.106992 5.491871 4.460293 5.510677 2.757941

25 H 8.970657 7.541154 6.257547 7.834072 4.706701

26 H 8.343101 6.963637 5.442738 7.443352 4.231608

27 H 8.109123 6.907534 5.444689 7.577053 4.224004

11 12 13 14 15

11 C 0.000000

12 C 1.531530 0.000000

13 C 2.545601 1.527316 0.000000

14 H 7.171265 8.367545 9.690013 0.000000

15 H 9.008715 10.465232 11.482023 3.943047 0.000000

16 H 5.653863 6.936311 8.096979 2.476919 4.787429

17 H 7.317551 8.654520 9.757134 2.518974 3.797859

18 H 6.153878 7.606500 8.594604 3.077908 3.530810

19 H 2.171828 2.806223 4.221411 5.976493 8.285788

20 H 2.169769 2.782415 4.211187 5.808332 8.473443

21 H 1.096564 2.157800 2.775755 7.272356 8.981210

22 H 1.096012 2.158549 2.766572 7.425056 8.837651

23 H 2.157124 1.096428 2.158208 8.480828 10.651218

24 H 2.158212 1.096346 2.158259 8.358881 10.775809

25 H 3.500167 2.180146 1.094158 10.538307 12.492245

26 H 2.815132 2.178465 1.094991 9.815171 11.511418

27 H 2.812775 2.178806 1.094905 9.918627 11.391792

16 17 18 19 20

16 H 0.000000

17 H 1.767055 0.000000

18 H 1.770397 1.772348 0.000000

19 H 5.164935 6.845663 5.887764 0.000000

20 H 4.489294 6.255771 5.548703 1.766859 0.000000

21 H 5.440909 7.043748 5.893323 3.073044 2.524313

22 H 6.029716 7.595532 6.243286 2.508925 3.071195

23 H 7.339968 9.067329 8.027023 2.573280 3.085959

24 H 6.873554 8.618447 7.763183 3.137297 2.558770

25 H 9.003994 10.696769 9.600274 4.906935 4.889990

26 H 8.000369 9.604632 8.461355 4.786987 4.446078

27 H 8.405442 10.010130 8.703382 4.435089 4.770753

21 22 23 24 25

21 H 0.000000

22 H 1.757549 0.000000

23 H 3.060732 2.511729 0.000000

24 H 2.503565 3.061827 1.754320 0.000000

25 H 3.781114 3.773549 2.501720 2.503122 0.000000

26 H 2.598273 3.128324 3.077303 2.523482 1.765888

27 H 3.139875 2.586008 2.525385 3.077562 1.765912

26 27

26 H 0.000000

27 H 1.765831 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.94D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.100759 -0.470923 -0.137096

2 6 0 -2.853589 0.128760 0.442891

3 8 0 -4.888950 0.123097 -0.839746

4 8 0 -4.253743 -1.779576 0.161918

5 6 0 -2.303496 -0.542434 1.686015

6 16 0 -1.589809 0.097534 -0.990355

7 6 0 -0.123794 0.703340 -0.241615

8 16 0 1.074500 -0.587783 0.090692

9 16 0 0.020013 2.310185 0.360287

10 6 0 2.680135 0.285771 -0.097787

11 6 0 3.836797 -0.704002 -0.012537

12 6 0 5.194728 -0.007718 -0.142134

13 6 0 6.366042 -0.985502 -0.073886

14 1 0 -3.052243 1.184924 0.620018

15 1 0 -5.061265 -2.085062 -0.284772

16 1 0 -1.398980 -0.026527 2.010785

17 1 0 -3.032078 -0.490076 2.501293

18 1 0 -2.060056 -1.590040 1.508080

19 1 0 2.668743 0.794824 -1.064204

20 1 0 2.754009 1.042878 0.683076

21 1 0 3.795691 -1.241836 0.942187

22 1 0 3.739059 -1.459025 -0.800972

23 1 0 5.229437 0.541952 -1.090190

24 1 0 5.294839 0.742067 0.651451

25 1 0 7.325423 -0.468504 -0.171266

26 1 0 6.377589 -1.526002 0.878338

27 1 0 6.309735 -1.730473 -0.874302

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3006265 0.1934663 0.1810239

Leave Link 202 at Sat Aug 17 17:49:39 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.3871332171 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0550036343 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.3321295828 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2320

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.12D-08

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 97

GePol: Fraction of low-weight points (<1% of avg) = 4.18%

GePol: Cavity surface area = 309.031 Ang\*\*2

GePol: Cavity volume = 320.307 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057690240 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.3263605588 Hartrees.

Leave Link 301 at Sat Aug 17 17:49:39 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:49:39 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:49:39 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000480 -0.000024 -0.000008 Ang= -0.06 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 17:49:39 2019, MaxMem= 1342177280 cpu: 2.7

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16147200.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.44D-15 for 2302.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.93D-15 for 1527 1171.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.66D-15 for 2302.

Iteration 1 A^-1\*A deviation from orthogonality is 5.18D-12 for 2111 892.

E= -1658.67698152549

DIIS: error= 1.63D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67698152549 IErMin= 1 ErrMin= 1.63D-04

ErrMax= 1.63D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.97D-05 BMatP= 2.97D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.63D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.428 Goal= None Shift= 0.000

Gap= 0.484 Goal= None Shift= 0.000

RMSDP=1.10D-05 MaxDP=4.13D-04 OVMax= 9.33D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.10D-05 CP: 1.00D+00

E= -1658.67699355780 Delta-E= -0.000012032310 Rises=F Damp=F

DIIS: error= 2.58D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67699355780 IErMin= 2 ErrMin= 2.58D-05

ErrMax= 2.58D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.60D-07 BMatP= 2.97D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.661D-01 0.107D+01

Coeff: -0.661D-01 0.107D+01

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.81D-06 MaxDP=7.63D-05 DE=-1.20D-05 OVMax= 1.35D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.67D-06 CP: 1.00D+00 1.06D+00

E= -1658.67699364111 Delta-E= -0.000000083316 Rises=F Damp=F

DIIS: error= 3.23D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67699364111 IErMin= 2 ErrMin= 2.58D-05

ErrMax= 3.23D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.66D-07 BMatP= 5.60D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.398D-01 0.545D+00 0.495D+00

Coeff: -0.398D-01 0.545D+00 0.495D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.16D-06 MaxDP=5.92D-05 DE=-8.33D-08 OVMax= 1.35D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 7.52D-07 CP: 1.00D+00 1.08D+00 4.83D-01

E= -1658.67699370339 Delta-E= -0.000000062273 Rises=F Damp=F

DIIS: error= 1.78D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67699370339 IErMin= 4 ErrMin= 1.78D-05

ErrMax= 1.78D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.39D-07 BMatP= 4.66D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.118D-01 0.155D+00 0.348D+00 0.510D+00

Coeff: -0.118D-01 0.155D+00 0.348D+00 0.510D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.26D-07 MaxDP=1.73D-05 DE=-6.23D-08 OVMax= 5.03D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.18D-07 CP: 1.00D+00 1.08D+00 6.20D-01 6.24D-01

E= -1658.67699372808 Delta-E= -0.000000024691 Rises=F Damp=F

DIIS: error= 1.30D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67699372808 IErMin= 5 ErrMin= 1.30D-06

ErrMax= 1.30D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.82D-09 BMatP= 1.39D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.310D-02 0.361D-01 0.130D+00 0.228D+00 0.609D+00

Coeff: -0.310D-02 0.361D-01 0.130D+00 0.228D+00 0.609D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=9.90D-08 MaxDP=5.64D-06 DE=-2.47D-08 OVMax= 6.38D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 7.09D-08 CP: 1.00D+00 1.08D+00 6.47D-01 6.59D-01 7.92D-01

E= -1658.67699372860 Delta-E= -0.000000000522 Rises=F Damp=F

DIIS: error= 6.63D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67699372860 IErMin= 6 ErrMin= 6.63D-07

ErrMax= 6.63D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.83D-10 BMatP= 2.82D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.653D-03-0.131D-01 0.402D-02 0.278D-01 0.315D+00 0.665D+00

Coeff: 0.653D-03-0.131D-01 0.402D-02 0.278D-01 0.315D+00 0.665D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.57D-08 MaxDP=1.49D-06 DE=-5.22D-10 OVMax= 3.34D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.62D-08 CP: 1.00D+00 1.08D+00 6.53D-01 6.75D-01 8.59D-01

CP: 8.52D-01

E= -1658.67699372869 Delta-E= -0.000000000089 Rises=F Damp=F

DIIS: error= 1.45D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67699372869 IErMin= 7 ErrMin= 1.45D-07

ErrMax= 1.45D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.17D-11 BMatP= 4.83D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.477D-03-0.821D-02-0.518D-02 0.764D-03 0.112D+00 0.309D+00

Coeff-Com: 0.591D+00

Coeff: 0.477D-03-0.821D-02-0.518D-02 0.764D-03 0.112D+00 0.309D+00

Coeff: 0.591D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.40D-08 MaxDP=5.40D-07 DE=-8.87D-11 OVMax= 1.27D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.11D-08 CP: 1.00D+00 1.08D+00 6.52D-01 6.77D-01 8.94D-01

CP: 8.92D-01 9.59D-01

E= -1658.67699372870 Delta-E= -0.000000000016 Rises=F Damp=F

DIIS: error= 4.02D-08 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67699372870 IErMin= 8 ErrMin= 4.02D-08

ErrMax= 4.02D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.40D-12 BMatP= 3.17D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.824D-04-0.108D-02-0.281D-02-0.445D-02-0.723D-02 0.140D-01

Coeff-Com: 0.257D+00 0.744D+00

Coeff: 0.824D-04-0.108D-02-0.281D-02-0.445D-02-0.723D-02 0.140D-01

Coeff: 0.257D+00 0.744D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=7.50D-09 MaxDP=2.96D-07 DE=-1.59D-11 OVMax= 1.18D-06

Error on total polarization charges = 0.04163

SCF Done: E(UB3LYP) = -1658.67699373 A.U. after 8 cycles

NFock= 8 Conv=0.75D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655235698980D+03 PE=-6.147420881661D+03 EE= 1.731181828393D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.62

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:49:58 2019, MaxMem= 1342177280 cpu: 211.3

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 337

Leave Link 701 at Sat Aug 17 17:49:59 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:49:59 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:50:02 2019, MaxMem= 1342177280 cpu: 38.7

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.40132431D+00-2.93307618D+00 6.55026915D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000014241 0.000008655 -0.000026941

2 6 -0.000009664 -0.000007496 0.000021848

3 8 0.000000511 0.000033621 0.000044215

4 8 0.000004847 0.000009825 -0.000015613

5 6 0.000002799 -0.000031169 -0.000004381

6 16 0.000018799 0.000036147 0.000017671

7 6 -0.000013260 0.000007436 0.000038000

8 16 0.000007409 0.000005418 -0.000009370

9 16 0.000005573 -0.000019499 0.000051519

10 6 -0.000005237 -0.000002473 0.000003644

11 6 -0.000000844 0.000005251 -0.000009878

12 6 0.000001798 0.000002706 -0.000003063

13 6 -0.000002879 0.000008471 -0.000015775

14 1 -0.000003484 -0.000015631 0.000036894

15 1 0.000000736 0.000027239 -0.000039870

16 1 0.000002570 -0.000042962 0.000001181

17 1 0.000003742 -0.000050684 -0.000011122

18 1 0.000000479 -0.000026174 -0.000039867

19 1 0.000003520 0.000028214 0.000029917

20 1 -0.000002197 -0.000018459 0.000034046

21 1 -0.000000939 -0.000012932 -0.000028602

22 1 0.000001378 0.000025619 -0.000026747

23 1 0.000000120 0.000026637 0.000021430

24 1 0.000000091 -0.000017712 0.000019286

25 1 0.000000912 0.000005158 -0.000012427

26 1 -0.000000439 -0.000014230 -0.000038221

27 1 -0.000002101 0.000029024 -0.000037772

-------------------------------------------------------------------

Cartesian Forces: Max 0.000051519 RMS 0.000021026

Leave Link 716 at Sat Aug 17 17:50:02 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000019555 RMS 0.000006051

Search for a local minimum.

Step number 43 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .60511D-05 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43

DE= -3.45D-06 DEPred=-8.15D-08 R= 4.23D+01

TightC=F SS= 1.41D+00 RLast= 7.00D-03 DXNew= 1.4142D-01 2.0992D-02

Trust test= 4.23D+01 RLast= 7.00D-03 DXMaxT set to 8.41D-02

ITU= 1 1 1 1 -1 -1 0 -1 -1 -1 0 -1 0 0 -1 -1 0 0 -1 0

ITU= 0 -1 1 -1 1 -1 1 1 -1 1 -1 1 1 -1 0 0 -1 0 0 -1

ITU= -1 0 0

Eigenvalues --- 0.00012 0.00211 0.00282 0.00335 0.00350

Eigenvalues --- 0.00370 0.00570 0.01165 0.01951 0.02331

Eigenvalues --- 0.03466 0.03561 0.03914 0.04298 0.04654

Eigenvalues --- 0.04805 0.04848 0.05236 0.05452 0.05473

Eigenvalues --- 0.05592 0.05638 0.05884 0.06251 0.08256

Eigenvalues --- 0.08350 0.09022 0.11044 0.12073 0.12219

Eigenvalues --- 0.13751 0.14525 0.15730 0.15960 0.16048

Eigenvalues --- 0.16070 0.16179 0.16313 0.17047 0.18234

Eigenvalues --- 0.20163 0.21733 0.21934 0.22399 0.23230

Eigenvalues --- 0.24813 0.25388 0.25596 0.25927 0.27965

Eigenvalues --- 0.28483 0.29010 0.29524 0.29711 0.29823

Eigenvalues --- 0.31397 0.33402 0.33578 0.33731 0.33880

Eigenvalues --- 0.33922 0.33993 0.33995 0.34049 0.34104

Eigenvalues --- 0.34227 0.34290 0.34649 0.34795 0.35114

Eigenvalues --- 0.36439 0.41706 0.52532 0.67025 0.94558

En-DIIS/RFO-DIIS IScMMF= 0 using points: 43 42 41 40 39

RFO step: Lambda=-5.63174336D-08.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 1.04D-05 SmlDif= 1.00D-05

RMS Error= 0.1673981576D-03 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 0.85460 -0.28811 -0.04357 0.46475 0.01232

Iteration 1 RMS(Cart)= 0.01020139 RMS(Int)= 0.00004441

Iteration 2 RMS(Cart)= 0.00006289 RMS(Int)= 0.00000014

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000014

ITry= 1 IFail=0 DXMaxC= 5.51D-02 DCOld= 1.00D+10 DXMaxT= 8.41D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83550 0.00000 0.00009 -0.00023 -0.00014 2.83536

R2 2.28947 -0.00001 -0.00023 0.00012 -0.00011 2.28937

R3 2.55315 0.00000 -0.00003 -0.00040 -0.00043 2.55271

R4 2.86495 0.00000 0.00010 0.00031 0.00040 2.86536

R5 3.61146 0.00001 -0.00045 -0.00042 -0.00087 3.61059

R6 2.05826 0.00000 0.00004 -0.00016 -0.00013 2.05813

R7 1.83697 0.00000 -0.00003 -0.00005 -0.00008 1.83689

R8 2.06126 0.00000 0.00006 0.00003 0.00009 2.06135

R9 2.06858 0.00000 -0.00004 0.00007 0.00004 2.06862

R10 2.06006 0.00000 0.00003 -0.00016 -0.00013 2.05993

R11 3.31474 -0.00001 -0.00004 0.00030 0.00026 3.31500

R12 3.38748 0.00000 0.00002 0.00008 0.00010 3.38758

R13 3.25391 -0.00001 -0.00025 0.00004 -0.00021 3.25370

R14 3.47252 0.00000 0.00021 -0.00048 -0.00027 3.47224

R15 2.88131 0.00000 -0.00007 0.00017 0.00009 2.88141

R16 2.06424 0.00000 -0.00004 -0.00002 -0.00006 2.06418

R17 2.06007 0.00000 0.00000 -0.00013 -0.00013 2.05994

R18 2.89417 0.00000 -0.00007 -0.00011 -0.00019 2.89399

R19 2.07220 0.00000 -0.00007 -0.00003 -0.00010 2.07211

R20 2.07116 0.00000 -0.00002 -0.00004 -0.00006 2.07110

R21 2.88621 0.00000 0.00002 -0.00013 -0.00011 2.88610

R22 2.07195 0.00000 -0.00007 -0.00006 -0.00013 2.07182

R23 2.07179 0.00000 -0.00001 -0.00001 -0.00002 2.07178

R24 2.06766 0.00000 -0.00003 -0.00003 -0.00006 2.06760

R25 2.06923 0.00000 -0.00009 0.00001 -0.00008 2.06915

R26 2.06907 0.00000 -0.00001 -0.00001 -0.00002 2.06905

A1 2.17604 -0.00001 0.00030 0.00001 0.00030 2.17634

A2 1.97761 -0.00001 -0.00023 0.00025 0.00002 1.97763

A3 2.12893 0.00002 -0.00005 -0.00022 -0.00026 2.12866

A4 2.02817 0.00000 0.00000 -0.00023 -0.00023 2.02794

A5 1.82682 0.00002 0.00039 0.00178 0.00217 1.82898

A6 1.87424 -0.00001 0.00004 -0.00005 -0.00001 1.87423

A7 1.94740 -0.00002 -0.00010 -0.00044 -0.00054 1.94686

A8 1.94135 0.00001 0.00008 -0.00068 -0.00059 1.94076

A9 1.83218 0.00001 -0.00044 -0.00026 -0.00070 1.83148

A10 1.87209 -0.00001 -0.00014 -0.00030 -0.00043 1.87166

A11 1.91307 0.00000 0.00025 -0.00035 -0.00010 1.91297

A12 1.92626 0.00000 0.00023 0.00001 0.00025 1.92650

A13 1.95265 -0.00001 -0.00033 -0.00006 -0.00039 1.95225

A14 1.88342 0.00000 0.00008 -0.00018 -0.00010 1.88332

A15 1.89435 0.00000 -0.00018 0.00019 0.00001 1.89436

A16 1.89248 0.00000 -0.00005 0.00039 0.00034 1.89282

A17 1.79971 -0.00001 -0.00029 -0.00078 -0.00107 1.79864

A18 1.97042 0.00002 0.00002 -0.00119 -0.00117 1.96924

A19 2.14278 -0.00001 -0.00007 0.00018 0.00010 2.14289

A20 2.15497 -0.00001 0.00016 0.00059 0.00076 2.15572

A21 1.79536 -0.00001 -0.00005 0.00052 0.00047 1.79584

A22 1.92679 0.00001 0.00018 -0.00025 -0.00007 1.92672

A23 1.87881 0.00000 0.00027 0.00040 0.00067 1.87948

A24 1.89220 -0.00001 -0.00023 -0.00008 -0.00031 1.89189

A25 1.93895 0.00000 0.00002 0.00004 0.00006 1.93901

A26 1.93840 -0.00001 -0.00015 -0.00010 -0.00025 1.93815

A27 1.88680 0.00000 -0.00009 0.00001 -0.00008 1.88672

A28 1.95278 0.00000 -0.00002 -0.00014 -0.00015 1.95262

A29 1.91626 0.00000 -0.00003 -0.00001 -0.00005 1.91621

A30 1.91699 0.00001 0.00017 0.00006 0.00023 1.91722

A31 1.90699 0.00000 -0.00014 0.00002 -0.00011 1.90688

A32 1.90857 0.00000 0.00003 -0.00004 -0.00001 1.90855

A33 1.85990 0.00000 -0.00001 0.00012 0.00011 1.86001

A34 1.96616 0.00000 0.00000 0.00010 0.00009 1.96626

A35 1.90621 0.00000 0.00007 -0.00007 0.00000 1.90621

A36 1.90777 0.00000 -0.00009 -0.00004 -0.00013 1.90764

A37 1.91273 0.00000 -0.00010 0.00023 0.00014 1.91286

A38 1.91288 0.00000 0.00015 -0.00028 -0.00013 1.91275

A39 1.85474 0.00000 -0.00004 0.00007 0.00003 1.85477

A40 1.94547 0.00000 0.00000 0.00000 0.00001 1.94548

A41 1.94223 0.00000 -0.00004 -0.00013 -0.00017 1.94207

A42 1.94280 0.00000 -0.00010 0.00030 0.00019 1.94299

A43 1.87694 0.00000 0.00008 -0.00012 -0.00004 1.87690

A44 1.87709 0.00000 -0.00007 0.00004 -0.00003 1.87705

A45 1.87592 0.00000 0.00014 -0.00010 0.00004 1.87596

D1 2.73411 0.00000 -0.00115 -0.01417 -0.01532 2.71879

D2 -1.39287 -0.00002 -0.00098 -0.01352 -0.01451 -1.40737

D3 0.54820 -0.00001 -0.00129 -0.01306 -0.01435 0.53385

D4 -0.44444 0.00000 -0.00047 -0.01291 -0.01338 -0.45782

D5 1.71177 -0.00001 -0.00030 -0.01226 -0.01257 1.69920

D6 -2.63035 0.00000 -0.00061 -0.01180 -0.01241 -2.64276

D7 -3.10028 0.00000 0.00002 0.00006 0.00009 -3.10019

D8 0.00549 0.00001 0.00069 0.00129 0.00198 0.00747

D9 3.13580 0.00000 0.00068 0.00266 0.00334 3.13914

D10 -1.07533 0.00000 0.00108 0.00224 0.00331 -1.07202

D11 1.03355 0.00000 0.00095 0.00270 0.00365 1.03720

D12 1.04352 0.00000 0.00024 0.00081 0.00105 1.04457

D13 3.11558 0.00000 0.00064 0.00038 0.00102 3.11660

D14 -1.05873 0.00000 0.00051 0.00084 0.00136 -1.05737

D15 -0.99602 0.00000 0.00080 0.00184 0.00264 -0.99338

D16 1.07604 0.00000 0.00120 0.00142 0.00262 1.07865

D17 -3.09827 0.00000 0.00107 0.00188 0.00296 -3.09532

D18 -3.07758 -0.00001 -0.00032 -0.00848 -0.00880 -3.08638

D19 -0.87027 -0.00001 -0.00012 -0.00782 -0.00794 -0.87820

D20 1.23444 -0.00001 -0.00035 -0.00903 -0.00938 1.22506

D21 1.82602 -0.00001 0.00053 -0.00190 -0.00137 1.82465

D22 -1.13591 -0.00002 -0.00013 0.00054 0.00041 -1.13550

D23 2.58821 0.00001 -0.00242 0.00942 0.00700 2.59521

D24 -0.73449 0.00001 -0.00179 0.00691 0.00512 -0.72937

D25 -3.02366 -0.00002 -0.00204 -0.00025 -0.00229 -3.02595

D26 -0.90458 -0.00001 -0.00174 -0.00010 -0.00184 -0.90642

D27 1.13259 -0.00001 -0.00183 0.00008 -0.00174 1.13084

D28 -3.12487 0.00001 0.00008 0.00145 0.00153 -3.12334

D29 -1.00440 0.00000 -0.00013 0.00138 0.00125 -1.00315

D30 1.03533 0.00001 -0.00006 0.00155 0.00149 1.03682

D31 1.07530 0.00000 -0.00039 0.00109 0.00070 1.07600

D32 -3.08741 0.00000 -0.00060 0.00102 0.00042 -3.08698

D33 -1.04768 0.00000 -0.00053 0.00119 0.00066 -1.04702

D34 -1.02544 0.00000 -0.00019 0.00112 0.00093 -1.02451

D35 1.09503 0.00000 -0.00040 0.00105 0.00065 1.09568

D36 3.13476 0.00000 -0.00033 0.00122 0.00089 3.13565

D37 -3.13100 -0.00001 0.00050 -0.00182 -0.00132 -3.13232

D38 -1.00130 0.00000 0.00042 -0.00151 -0.00108 -1.00238

D39 1.02118 0.00000 0.00036 -0.00149 -0.00112 1.02005

D40 1.02637 0.00000 0.00065 -0.00173 -0.00108 1.02529

D41 -3.12711 0.00000 0.00057 -0.00142 -0.00084 -3.12796

D42 -1.10463 0.00000 0.00052 -0.00140 -0.00088 -1.10552

D43 -1.00318 0.00000 0.00072 -0.00186 -0.00114 -1.00431

D44 1.12652 0.00000 0.00065 -0.00155 -0.00090 1.12562

D45 -3.13418 0.00000 0.00059 -0.00153 -0.00094 -3.13513

D46 3.13871 0.00000 0.00125 -0.00300 -0.00175 3.13696

D47 -1.04924 0.00000 0.00133 -0.00324 -0.00191 -1.05115

D48 1.04290 0.00000 0.00141 -0.00325 -0.00184 1.04106

D49 1.01270 0.00000 0.00123 -0.00314 -0.00191 1.01079

D50 3.10793 0.00000 0.00131 -0.00337 -0.00207 3.10586

D51 -1.08311 0.00000 0.00139 -0.00339 -0.00200 -1.08511

D52 -1.01636 0.00000 0.00125 -0.00319 -0.00195 -1.01831

D53 1.07888 0.00000 0.00132 -0.00343 -0.00211 1.07677

D54 -3.11217 0.00000 0.00140 -0.00344 -0.00204 -3.11421

Item Value Threshold Converged?

Maximum Force 0.000020 0.000450 YES

RMS Force 0.000006 0.000300 YES

Maximum Displacement 0.055088 0.001800 NO

RMS Displacement 0.010214 0.001200 NO

Predicted change in Energy=-6.950565D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:50:02 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.093992 -0.409587 -0.208017

2 6 0 -2.845317 0.074642 0.468410

3 8 0 -4.886347 0.302601 -0.784773

4 8 0 -4.244805 -1.750936 -0.155068

5 6 0 -2.300486 -0.804933 1.576839

6 16 0 -1.577098 0.289463 -0.944396

7 6 0 -0.116270 0.763692 -0.096820

8 16 0 1.082879 -0.563799 0.018659

9 16 0 0.019366 2.245352 0.769680

10 6 0 2.687784 0.330686 0.000526

11 6 0 3.846299 -0.657995 -0.072205

12 6 0 5.203417 0.051536 -0.063284

13 6 0 6.376953 -0.922137 -0.148645

14 1 0 -3.040044 1.084504 0.826782

15 1 0 -5.053649 -1.969544 -0.647861

16 1 0 -1.396160 -0.355709 1.989485

17 1 0 -3.031549 -0.894407 2.386674

18 1 0 -2.058090 -1.805573 1.218772

19 1 0 2.685827 0.998355 -0.863981

20 1 0 2.750958 0.942279 0.900653

21 1 0 3.795642 -1.352256 0.775010

22 1 0 3.760276 -1.265911 -0.980062

23 1 0 5.248007 0.755695 -0.902434

24 1 0 5.291260 0.654142 0.848366

25 1 0 7.335691 -0.394953 -0.145553

26 1 0 6.379452 -1.616452 0.698015

27 1 0 6.332155 -1.520391 -1.064549

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.500407 0.000000

3 O 1.211481 2.405876 0.000000

4 O 1.350838 2.383280 2.241677 0.000000

5 C 2.560991 1.516281 3.672945 2.770343 0.000000

6 S 2.713979 1.910641 3.313123 3.450062 2.842115

7 C 4.148641 2.870884 4.841438 4.834413 3.167415

8 S 5.184125 4.005072 6.085048 5.461107 3.732723

9 S 4.992424 3.606820 5.500602 5.916808 3.916306

10 C 6.825246 5.558748 7.614785 7.240038 5.353245

11 C 7.945337 6.753277 8.814171 8.165008 6.365838

12 C 9.309962 8.066309 10.118642 9.619055 7.728654

13 C 10.483650 9.296482 11.347536 10.654046 8.848106

14 H 2.100934 1.089115 2.572416 3.233450 2.163216

15 H 1.883579 3.209593 2.282406 0.972041 3.726328

16 H 3.479973 2.144511 4.506805 3.828909 1.090818

17 H 2.845392 2.157192 3.864089 2.943821 1.094665

18 H 2.851210 2.172090 4.056801 2.583050 1.090068

19 H 6.955468 5.763858 7.604484 7.489647 5.837188

20 H 7.064704 5.679606 7.847184 7.570248 5.387677

21 H 8.006328 6.799439 8.974876 8.103874 6.172945

22 H 7.938442 6.894128 8.789907 8.062083 6.594170

23 H 9.439971 8.236804 10.145161 9.846585 8.097043

24 H 9.504231 8.166031 10.313797 9.885738 7.764932

25 H 11.429863 10.210308 12.258606 11.659617 9.797480

26 H 10.581609 9.381305 11.523874 10.659300 8.761975

27 H 10.520079 9.440343 11.369097 10.618493 9.056008

6 7 8 9 10

6 S 0.000000

7 C 1.754223 0.000000

8 S 2.954828 1.792630 0.000000

9 S 3.051598 1.721783 3.096195 0.000000

10 C 4.368501 2.838959 1.837432 3.373129 0.000000

11 C 5.574194 4.209959 2.766518 4.876845 1.524774

12 C 6.841663 5.367248 4.167036 5.690434 2.531877

13 C 8.085056 6.708699 5.308825 7.162068 3.898946

14 H 2.430920 3.082924 4.513143 3.272738 5.836005

15 H 4.156616 5.670268 6.330667 6.746128 8.101929

16 H 3.009426 2.691440 3.173814 3.202679 4.594094

17 H 3.822696 4.173235 4.758709 4.666995 6.317067

18 H 3.049562 3.478875 3.584405 4.574658 5.345189

19 H 4.322213 2.914678 2.405997 3.366581 1.092318

20 H 4.749994 3.041027 2.414265 3.029315 1.090076

21 H 5.875196 4.532149 2.924519 5.215656 2.158580

22 H 5.559498 4.463968 2.942594 5.420791 2.158915

23 H 6.841140 5.424440 4.465174 5.688034 2.747856

24 H 7.107835 5.490606 4.458954 5.507359 2.757089

25 H 8.974653 7.541654 6.257247 7.831825 4.706477

26 H 8.344862 6.963566 5.442728 7.441059 4.231577

27 H 8.114573 6.909103 5.444567 7.576049 4.224016

11 12 13 14 15

11 C 0.000000

12 C 1.531431 0.000000

13 C 2.545550 1.527256 0.000000

14 H 7.160042 8.355470 9.677701 0.000000

15 H 9.014467 10.470620 11.489340 3.944159 0.000000

16 H 5.641394 6.923448 8.081691 2.475569 4.789288

17 H 7.307994 8.643597 9.744153 2.519806 3.801738

18 H 6.151859 7.604078 8.590706 3.077407 3.533353

19 H 2.171889 2.806393 4.221896 5.970904 8.291840

20 H 2.169585 2.781573 4.210096 5.793219 8.472810

21 H 1.096511 2.157591 2.775123 7.257208 8.984183

22 H 1.095978 2.158427 2.767027 7.418456 8.848205

23 H 2.156986 1.096359 2.158203 8.472904 10.659074

24 H 2.158024 1.096338 2.158105 8.342439 10.776807

25 H 3.500061 2.180072 1.094126 10.525688 12.499096

26 H 2.815802 2.178260 1.094949 9.799931 11.517459

27 H 2.812108 2.178884 1.094895 9.909628 11.402276

16 17 18 19 20

16 H 0.000000

17 H 1.767046 0.000000

18 H 1.770382 1.772523 0.000000

19 H 5.161238 6.843807 5.891062 0.000000

20 H 4.479835 6.246524 5.547867 1.766726 0.000000

21 H 5.424284 7.029766 5.888004 3.073003 2.524290

22 H 6.019594 7.589586 6.243355 2.508947 3.071142

23 H 7.330988 9.060471 8.027370 2.573933 3.085643

24 H 6.858829 8.604275 7.758888 3.136701 2.557125

25 H 8.989169 10.683693 9.596580 4.907003 4.889019

26 H 7.982325 9.588528 8.455712 4.787475 4.444562

27 H 8.391094 9.999087 8.700063 4.436216 4.769877

21 22 23 24 25

21 H 0.000000

22 H 1.757551 0.000000

23 H 3.060498 2.511228 0.000000

24 H 2.503575 3.061645 1.754276 0.000000

25 H 3.780981 3.773403 2.501057 2.503632 0.000000

26 H 2.598424 3.130321 3.077124 2.522374 1.765803

27 H 3.137857 2.585819 2.526307 3.077548 1.765857

26 27

26 H 0.000000

27 H 1.765813 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.12D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.103159 -0.464994 -0.130810

2 6 0 -2.848929 0.121805 0.446940

3 8 0 -4.899598 0.143825 -0.811038

4 8 0 -4.254339 -1.778965 0.143758

5 6 0 -2.295931 -0.563976 1.681042

6 16 0 -1.591712 0.098347 -0.991602

7 6 0 -0.123998 0.703106 -0.245023

8 16 0 1.075240 -0.589416 0.078612

9 16 0 0.019304 2.307108 0.364221

10 6 0 2.680479 0.286827 -0.099043

11 6 0 3.837807 -0.702482 -0.016596

12 6 0 5.195369 -0.003736 -0.135176

13 6 0 6.367627 -0.980353 -0.067775

14 1 0 -3.040244 1.177300 0.635355

15 1 0 -5.067154 -2.074324 -0.300042

16 1 0 -1.388132 -0.054553 2.007035

17 1 0 -3.020669 -0.517319 2.500109

18 1 0 -2.056941 -1.610413 1.491043

19 1 0 2.672129 0.802807 -1.061776

20 1 0 2.751075 1.038354 0.687397

21 1 0 3.793392 -1.247443 0.933868

22 1 0 3.744303 -1.451614 -0.811093

23 1 0 5.233785 0.552329 -1.079272

24 1 0 5.290718 0.740781 0.663923

25 1 0 7.326669 -0.461673 -0.158988

26 1 0 6.376363 -1.525559 0.881744

27 1 0 6.315290 -1.721359 -0.872117

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3048504 0.1933993 0.1809198

Leave Link 202 at Sat Aug 17 17:50:02 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.3953854377 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0550075720 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.3403778658 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2323

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.12D-08

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 94

GePol: Fraction of low-weight points (<1% of avg) = 4.05%

GePol: Cavity surface area = 309.090 Ang\*\*2

GePol: Cavity volume = 320.329 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057825101 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.3345953556 Hartrees.

Leave Link 301 at Sat Aug 17 17:50:02 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:50:02 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:50:02 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999996 -0.002909 -0.000154 -0.000043 Ang= -0.33 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.63021089843

Leave Link 401 at Sat Aug 17 17:50:03 2019, MaxMem= 1342177280 cpu: 7.7

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16188987.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.88D-15 for 2323.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.36D-15 for 956 38.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.11D-15 for 2323.

Iteration 1 A^-1\*A deviation from orthogonality is 9.28D-12 for 773 715.

E= -1658.67659135986

DIIS: error= 9.91D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67659135986 IErMin= 1 ErrMin= 9.91D-04

ErrMax= 9.91D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.03D-03 BMatP= 1.03D-03

IDIUse=3 WtCom= 9.90D-01 WtEn= 9.91D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.428 Goal= None Shift= 0.000

Gap= 0.484 Goal= None Shift= 0.000

RMSDP=6.46D-05 MaxDP=2.39D-03 OVMax= 5.52D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 6.46D-05 CP: 1.00D+00

E= -1658.67700747371 Delta-E= -0.000416113853 Rises=F Damp=F

DIIS: error= 1.53D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67700747371 IErMin= 2 ErrMin= 1.53D-04

ErrMax= 1.53D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.98D-05 BMatP= 1.03D-03

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.53D-03

Coeff-Com: -0.662D-01 0.107D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.661D-01 0.107D+01

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.08D-05 MaxDP=4.73D-04 DE=-4.16D-04 OVMax= 8.17D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.00D-05 CP: 1.00D+00 1.06D+00

E= -1658.67700997306 Delta-E= -0.000002499348 Rises=F Damp=F

DIIS: error= 1.99D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67700997306 IErMin= 2 ErrMin= 1.53D-04

ErrMax= 1.99D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.85D-05 BMatP= 1.98D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.99D-03

Coeff-Com: -0.413D-01 0.563D+00 0.479D+00

Coeff-En: 0.000D+00 0.215D+00 0.785D+00

Coeff: -0.413D-01 0.562D+00 0.479D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=7.18D-06 MaxDP=3.88D-04 DE=-2.50D-06 OVMax= 8.15D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 4.54D-06 CP: 1.00D+00 1.08D+00 4.53D-01

E= -1658.67701255244 Delta-E= -0.000002579384 Rises=F Damp=F

DIIS: error= 1.01D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67701255244 IErMin= 4 ErrMin= 1.01D-04

ErrMax= 1.01D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.83D-06 BMatP= 1.85D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.01D-03

Coeff-Com: -0.114D-01 0.151D+00 0.334D+00 0.526D+00

Coeff-En: 0.000D+00 0.000D+00 0.244D+00 0.756D+00

Coeff: -0.114D-01 0.151D+00 0.334D+00 0.527D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.51D-06 MaxDP=9.96D-05 DE=-2.58D-06 OVMax= 2.83D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.21D-06 CP: 1.00D+00 1.08D+00 6.01D-01 6.47D-01

E= -1658.67701342108 Delta-E= -0.000000868643 Rises=F Damp=F

DIIS: error= 5.96D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67701342108 IErMin= 5 ErrMin= 5.96D-06

ErrMax= 5.96D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.06D-08 BMatP= 4.83D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.255D-02 0.286D-01 0.111D+00 0.209D+00 0.654D+00

Coeff: -0.255D-02 0.286D-01 0.111D+00 0.209D+00 0.654D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.71D-07 MaxDP=3.43D-05 DE=-8.69D-07 OVMax= 4.07D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 4.15D-07 CP: 1.00D+00 1.08D+00 6.28D-01 6.79D-01 7.98D-01

E= -1658.67701343482 Delta-E= -0.000000013736 Rises=F Damp=F

DIIS: error= 3.47D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67701343482 IErMin= 6 ErrMin= 3.47D-06

ErrMax= 3.47D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.55D-08 BMatP= 7.06D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.722D-03-0.139D-01 0.101D-02 0.225D-01 0.345D+00 0.645D+00

Coeff: 0.722D-03-0.139D-01 0.101D-02 0.225D-01 0.345D+00 0.645D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.13D-07 MaxDP=9.54D-06 DE=-1.37D-08 OVMax= 1.86D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.48D-07 CP: 1.00D+00 1.08D+00 6.31D-01 6.97D-01 8.81D-01

CP: 8.24D-01

E= -1658.67701343819 Delta-E= -0.000000003367 Rises=F Damp=F

DIIS: error= 7.62D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67701343819 IErMin= 7 ErrMin= 7.62D-07

ErrMax= 7.62D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.36D-10 BMatP= 1.55D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.465D-03-0.798D-02-0.516D-02-0.192D-03 0.124D+00 0.298D+00

Coeff-Com: 0.591D+00

Coeff: 0.465D-03-0.798D-02-0.516D-02-0.192D-03 0.124D+00 0.298D+00

Coeff: 0.591D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=8.43D-08 MaxDP=3.57D-06 DE=-3.37D-09 OVMax= 9.11D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 6.95D-08 CP: 1.00D+00 1.08D+00 6.31D-01 6.97D-01 9.15D-01

CP: 8.76D-01 9.22D-01

E= -1658.67701343838 Delta-E= -0.000000000195 Rises=F Damp=F

DIIS: error= 2.88D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67701343838 IErMin= 8 ErrMin= 2.88D-07

ErrMax= 2.88D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.92D-10 BMatP= 9.36D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.876D-04-0.117D-02-0.273D-02-0.445D-02-0.520D-02 0.225D-01

Coeff-Com: 0.306D+00 0.685D+00

Coeff: 0.876D-04-0.117D-02-0.273D-02-0.445D-02-0.520D-02 0.225D-01

Coeff: 0.306D+00 0.685D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.48D-08 MaxDP=1.74D-06 DE=-1.95D-10 OVMax= 6.42D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.67D-08 CP: 1.00D+00 1.08D+00 6.32D-01 7.00D-01 9.19D-01

CP: 9.23D-01 1.08D+00 8.38D-01

E= -1658.67701343846 Delta-E= -0.000000000080 Rises=F Damp=F

DIIS: error= 1.57D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67701343846 IErMin= 9 ErrMin= 1.57D-07

ErrMax= 1.57D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.65D-11 BMatP= 1.92D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.339D-04 0.830D-03-0.737D-03-0.284D-02-0.274D-01-0.420D-01

Coeff-Com: 0.837D-01 0.441D+00 0.548D+00

Coeff: -0.339D-04 0.830D-03-0.737D-03-0.284D-02-0.274D-01-0.420D-01

Coeff: 0.837D-01 0.441D+00 0.548D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.32D-08 MaxDP=1.08D-06 DE=-8.05D-11 OVMax= 2.61D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.00D-08 CP: 1.00D+00 1.08D+00 6.32D-01 7.00D-01 9.23D-01

CP: 9.43D-01 1.15D+00 1.04D+00 8.00D-01

E= -1658.67701343844 Delta-E= 0.000000000025 Rises=F Damp=F

DIIS: error= 5.93D-08 at cycle 10 NSaved= 10.

NSaved=10 IEnMin= 9 EnMin= -1658.67701343846 IErMin=10 ErrMin= 5.93D-08

ErrMax= 5.93D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.15D-12 BMatP= 6.65D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.373D-04 0.712D-03 0.192D-03-0.603D-03-0.135D-01-0.273D-01

Coeff-Com: -0.250D-01 0.931D-01 0.272D+00 0.701D+00

Coeff: -0.373D-04 0.712D-03 0.192D-03-0.603D-03-0.135D-01-0.273D-01

Coeff: -0.250D-01 0.931D-01 0.272D+00 0.701D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=9.92D-09 MaxDP=3.65D-07 DE= 2.46D-11 OVMax= 1.58D-06

Error on total polarization charges = 0.04162

SCF Done: E(UB3LYP) = -1658.67701344 A.U. after 10 cycles

NFock= 10 Conv=0.99D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655237827290D+03 PE=-6.147436260644D+03 EE= 1.731186824559D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.63

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:50:25 2019, MaxMem= 1342177280 cpu: 258.3

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 340

Leave Link 701 at Sat Aug 17 17:50:26 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:50:27 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:50:30 2019, MaxMem= 1342177280 cpu: 38.7

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.40968771D+00-2.94047615D+00 6.44713291D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000091643 0.000120667 0.000154378

2 6 0.000131216 0.000026023 0.000114160

3 8 0.000004020 0.000138882 -0.000040063

4 8 0.000074807 -0.000158158 -0.000054188

5 6 -0.000046896 -0.000008660 -0.000047700

6 16 -0.000010390 0.000059022 -0.000025534

7 6 -0.000024487 -0.000020808 0.000023102

8 16 0.000064823 -0.000006357 -0.000009500

9 16 0.000037632 -0.000008042 0.000057374

10 6 0.000008708 -0.000043603 0.000010517

11 6 -0.000028918 0.000028172 -0.000004764

12 6 0.000023256 0.000019573 0.000013834

13 6 0.000017044 -0.000001079 -0.000024156

14 1 -0.000063829 -0.000010534 0.000012747

15 1 -0.000040371 -0.000029174 -0.000037853

16 1 -0.000021869 -0.000049626 -0.000030826

17 1 -0.000005674 -0.000048444 -0.000022124

18 1 0.000016578 -0.000081819 -0.000038437

19 1 -0.000018570 0.000029487 -0.000008045

20 1 -0.000010457 0.000017481 0.000072011

21 1 -0.000007968 -0.000032832 -0.000004755

22 1 -0.000016418 0.000010169 -0.000039090

23 1 0.000004403 0.000047652 -0.000018680

24 1 0.000008080 -0.000003051 0.000019773

25 1 0.000014361 0.000022335 -0.000013802

26 1 -0.000000152 -0.000040633 -0.000018314

27 1 -0.000017286 0.000023355 -0.000040067

-------------------------------------------------------------------

Cartesian Forces: Max 0.000158158 RMS 0.000049593

Leave Link 716 at Sat Aug 17 17:50:30 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000215152 RMS 0.000043434

Search for a local minimum.

Step number 44 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .43434D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43 44

DE= -1.97D-05 DEPred=-6.95D-07 R= 2.84D+01

TightC=F SS= 1.41D+00 RLast= 3.99D-02 DXNew= 1.4142D-01 1.1968D-01

Trust test= 2.84D+01 RLast= 3.99D-02 DXMaxT set to 1.20D-01

ITU= 1 1 1 1 1 -1 -1 0 -1 -1 -1 0 -1 0 0 -1 -1 0 0 -1

ITU= 0 0 -1 1 -1 1 -1 1 1 -1 1 -1 1 1 -1 0 0 -1 0 0

ITU= -1 -1 0 0

Eigenvalues --- -1.26180 -0.44225 0.00000 0.00096 0.00208

Eigenvalues --- 0.00297 0.00328 0.00379 0.00593 0.00859

Eigenvalues --- 0.01653 0.02285 0.03500 0.03539 0.03925

Eigenvalues --- 0.04655 0.04759 0.04808 0.05011 0.05244

Eigenvalues --- 0.05433 0.05495 0.05556 0.05808 0.06230

Eigenvalues --- 0.07990 0.08314 0.08421 0.10742 0.10977

Eigenvalues --- 0.11988 0.12112 0.14020 0.14625 0.15473

Eigenvalues --- 0.15849 0.16030 0.16045 0.16203 0.16492

Eigenvalues --- 0.17699 0.18621 0.20311 0.21532 0.21910

Eigenvalues --- 0.22245 0.22749 0.23320 0.24842 0.25524

Eigenvalues --- 0.26024 0.27213 0.28685 0.29259 0.29548

Eigenvalues --- 0.29702 0.31132 0.31672 0.31980 0.33449

Eigenvalues --- 0.33877 0.33886 0.33933 0.33976 0.34006

Eigenvalues --- 0.34032 0.34116 0.34203 0.34259 0.34476

Eigenvalues --- 0.34720 0.34983 0.45071 0.52272 0.73893

Eigenvalue 1 is -1.26D+00 should be greater than 0.000000 Eigenvector:

R3 R2 A18 A3 A20

1 -0.43695 -0.32673 -0.30988 -0.29195 0.21360

A1 A4 A10 R18 R5

1 0.16110 0.15780 -0.15163 -0.14705 -0.14471

Eigenvalue 2 is -4.42D-01 should be greater than 0.000000 Eigenvector:

D22 A17 A21 D23 R2

1 -0.36633 0.35221 -0.30197 -0.23580 -0.21787

D24 D19 A10 A20 D25

1 0.20123 -0.16860 0.16434 -0.15678 -0.15484

Eigenvalue 3 is 1.34D-09 Eigenvector:

D1 D2 D3 D4 D5

1 -0.38570 -0.36360 -0.36214 -0.33297 -0.31088

D6 D20 D18 D19 D23

1 -0.30942 -0.23912 -0.22456 -0.20016 0.17493

Use linear search instead of GDIIS.

RFO step: Lambda=-1.26179891D+00 EMin=-1.26179876D+00

I= 1 Eig= -1.26D+00 Dot1= -1.34D-04

I= 1 Stepn= -2.99D-01 RXN= 2.99D-01 EDone=F

I= 2 Eig= -4.42D-01 Dot1= 2.50D-05

I= 2 Stepn= 1.50D-01 RXN= 3.35D-01 EDone=F

Mixed 2 eigenvectors in step. Raw Step.Grad= 1.59D-04.

RFO eigenvector is Hessian eigenvector with negative curvature.

Taking step of 3.35D-01 in eigenvector direction(s). Step.Grad= -8.99D-06.

Skip linear search -- no minimum in search direction.

Maximum step size ( 0.120) exceeded in Quadratic search.

-- Step size not scaled.

Iteration 1 RMS(Cart)= 0.16191762 RMS(Int)= 0.00636922

Iteration 2 RMS(Cart)= 0.02220789 RMS(Int)= 0.00034454

Iteration 3 RMS(Cart)= 0.00026200 RMS(Int)= 0.00032825

Iteration 4 RMS(Cart)= 0.00000005 RMS(Int)= 0.00032825

ITry= 1 IFail=0 DXMaxC= 5.78D-01 DCOld= 1.00D+10 DXMaxT= 1.20D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83536 0.00002 0.00000 0.01377 0.01377 2.84913

R2 2.28937 0.00009 0.00000 0.06516 0.06516 2.35453

R3 2.55271 0.00022 0.00000 0.12816 0.12816 2.68087

R4 2.86536 -0.00007 0.00000 -0.04744 -0.04744 2.81792

R5 3.61059 0.00006 0.00000 0.03077 0.03077 3.64135

R6 2.05813 0.00001 0.00000 0.00472 0.00472 2.06285

R7 1.83689 0.00005 0.00000 0.02932 0.02932 1.86621

R8 2.06135 -0.00004 0.00000 -0.02372 -0.02372 2.03763

R9 2.06862 0.00000 0.00000 -0.00024 -0.00024 2.06837

R10 2.05993 0.00006 0.00000 0.03590 0.03590 2.09582

R11 3.31500 0.00005 0.00000 0.03473 0.03473 3.34973

R12 3.38758 0.00003 0.00000 0.01408 0.01408 3.40166

R13 3.25370 0.00000 0.00000 0.01488 0.01488 3.26858

R14 3.47224 -0.00001 0.00000 -0.00506 -0.00506 3.46718

R15 2.88141 -0.00001 0.00000 -0.00640 -0.00640 2.87501

R16 2.06418 0.00003 0.00000 0.02094 0.02094 2.08512

R17 2.05994 0.00006 0.00000 0.03394 0.03394 2.09388

R18 2.89399 0.00006 0.00000 0.04150 0.04150 2.93549

R19 2.07211 0.00003 0.00000 0.02239 0.02239 2.09450

R20 2.07110 0.00002 0.00000 0.01382 0.01382 2.08492

R21 2.88610 0.00003 0.00000 0.01938 0.01938 2.90548

R22 2.07182 0.00004 0.00000 0.02995 0.02995 2.10177

R23 2.07178 0.00001 0.00000 0.00724 0.00724 2.07902

R24 2.06760 0.00002 0.00000 0.01428 0.01428 2.08188

R25 2.06915 0.00003 0.00000 0.02306 0.02306 2.09222

R26 2.06905 0.00001 0.00000 0.00345 0.00345 2.07250

A1 2.17634 -0.00006 0.00000 -0.04128 -0.04179 2.13456

A2 1.97763 -0.00005 0.00000 -0.02901 -0.02962 1.94801

A3 2.12866 0.00011 0.00000 0.06835 0.06761 2.19627

A4 2.02794 -0.00006 0.00000 -0.04432 -0.04421 1.98373

A5 1.82898 0.00003 0.00000 0.00567 0.00559 1.83457

A6 1.87423 -0.00003 0.00000 -0.01957 -0.01908 1.85514

A7 1.94686 -0.00001 0.00000 0.00656 0.00601 1.95287

A8 1.94076 0.00006 0.00000 0.04285 0.04231 1.98306

A9 1.83148 0.00001 0.00000 0.01117 0.01062 1.84210

A10 1.87166 0.00008 0.00000 0.06995 0.06995 1.94161

A11 1.91297 -0.00003 0.00000 -0.02255 -0.02257 1.89039

A12 1.92650 -0.00002 0.00000 -0.01683 -0.01689 1.90962

A13 1.95225 0.00003 0.00000 0.02891 0.02905 1.98130

A14 1.88332 0.00002 0.00000 0.01727 0.01703 1.90035

A15 1.89436 0.00000 0.00000 -0.00152 -0.00136 1.89301

A16 1.89282 0.00000 0.00000 -0.00509 -0.00498 1.88784

A17 1.79864 0.00007 0.00000 0.05445 0.05445 1.85308

A18 1.96924 0.00017 0.00000 0.10778 0.10756 2.07680

A19 2.14289 -0.00003 0.00000 -0.01420 -0.01437 2.12852

A20 2.15572 -0.00013 0.00000 -0.08736 -0.08764 2.06809

A21 1.79584 -0.00011 0.00000 -0.06591 -0.06591 1.72992

A22 1.92672 0.00002 0.00000 0.00148 0.00150 1.92822

A23 1.87948 -0.00004 0.00000 -0.02969 -0.02964 1.84984

A24 1.89189 0.00000 0.00000 0.01174 0.01176 1.90365

A25 1.93901 0.00003 0.00000 0.02011 0.02010 1.95910

A26 1.93815 -0.00002 0.00000 -0.00617 -0.00620 1.93196

A27 1.88672 0.00000 0.00000 0.00171 0.00171 1.88843

A28 1.95262 0.00002 0.00000 0.02054 0.02055 1.97318

A29 1.91621 -0.00002 0.00000 -0.01346 -0.01358 1.90264

A30 1.91722 0.00000 0.00000 -0.00909 -0.00912 1.90810

A31 1.90688 0.00001 0.00000 0.00499 0.00505 1.91193

A32 1.90855 -0.00001 0.00000 -0.00491 -0.00485 1.90370

A33 1.86001 0.00000 0.00000 0.00103 0.00094 1.86095

A34 1.96626 -0.00002 0.00000 -0.01163 -0.01163 1.95463

A35 1.90621 0.00000 0.00000 -0.00070 -0.00071 1.90550

A36 1.90764 0.00001 0.00000 0.01275 0.01275 1.92039

A37 1.91286 0.00001 0.00000 0.00421 0.00420 1.91706

A38 1.91275 0.00000 0.00000 -0.00171 -0.00167 1.91108

A39 1.85477 0.00000 0.00000 -0.00235 -0.00237 1.85241

A40 1.94548 -0.00001 0.00000 -0.00547 -0.00548 1.93999

A41 1.94207 0.00001 0.00000 0.00796 0.00798 1.95004

A42 1.94299 -0.00002 0.00000 -0.01129 -0.01129 1.93170

A43 1.87690 0.00000 0.00000 0.00180 0.00181 1.87872

A44 1.87705 0.00001 0.00000 0.00943 0.00940 1.88645

A45 1.87596 0.00000 0.00000 -0.00186 -0.00184 1.87412

D1 2.71879 0.00003 0.00000 0.03277 0.03240 2.75119

D2 -1.40737 0.00000 0.00000 0.01702 0.01657 -1.39080

D3 0.53385 0.00001 0.00000 0.02413 0.02314 0.55699

D4 -0.45782 -0.00003 0.00000 -0.02803 -0.02719 -0.48501

D5 1.69920 -0.00005 0.00000 -0.04378 -0.04302 1.65618

D6 -2.64276 -0.00004 0.00000 -0.03667 -0.03645 -2.67921

D7 -3.10019 0.00002 0.00000 0.01669 0.01838 -3.08181

D8 0.00747 -0.00004 0.00000 -0.04465 -0.04634 -0.03887

D9 3.13914 0.00001 0.00000 0.00150 0.00164 3.14078

D10 -1.07202 0.00001 0.00000 -0.00150 -0.00114 -1.07316

D11 1.03720 0.00001 0.00000 -0.00013 0.00014 1.03734

D12 1.04457 0.00002 0.00000 0.02149 0.02155 1.06612

D13 3.11660 0.00002 0.00000 0.01850 0.01877 3.13536

D14 -1.05737 0.00002 0.00000 0.01986 0.02005 -1.03732

D15 -0.99338 -0.00003 0.00000 -0.02393 -0.02447 -1.01785

D16 1.07865 -0.00003 0.00000 -0.02692 -0.02726 1.05139

D17 -3.09532 -0.00003 0.00000 -0.02556 -0.02597 -3.12129

D18 -3.08638 -0.00003 0.00000 -0.01998 -0.01983 -3.10621

D19 -0.87820 -0.00008 0.00000 -0.06704 -0.06705 -0.94526

D20 1.22506 -0.00001 0.00000 -0.00501 -0.00516 1.21991

D21 1.82465 -0.00005 0.00000 -0.03278 -0.03217 1.79248

D22 -1.13550 -0.00007 0.00000 -0.06084 -0.06145 -1.19695

D23 2.59521 -0.00004 0.00000 -0.04177 -0.04117 2.55404

D24 -0.72937 0.00000 0.00000 -0.00445 -0.00505 -0.73442

D25 -3.02595 -0.00006 0.00000 -0.03999 -0.04000 -3.06595

D26 -0.90642 -0.00004 0.00000 -0.03321 -0.03316 -0.93958

D27 1.13084 -0.00006 0.00000 -0.04086 -0.04090 1.08995

D28 -3.12334 -0.00002 0.00000 -0.02286 -0.02285 3.13699

D29 -1.00315 -0.00001 0.00000 -0.01212 -0.01220 -1.01534

D30 1.03682 -0.00002 0.00000 -0.02410 -0.02407 1.01275

D31 1.07600 0.00000 0.00000 0.00036 0.00040 1.07641

D32 -3.08698 0.00001 0.00000 0.01110 0.01105 -3.07593

D33 -1.04702 -0.00001 0.00000 -0.00089 -0.00082 -1.04784

D34 -1.02451 -0.00001 0.00000 -0.01117 -0.01116 -1.03567

D35 1.09568 -0.00001 0.00000 -0.00043 -0.00051 1.09518

D36 3.13565 -0.00002 0.00000 -0.01241 -0.01238 3.12327

D37 -3.13232 -0.00001 0.00000 -0.00375 -0.00374 -3.13606

D38 -1.00238 -0.00001 0.00000 -0.00670 -0.00666 -1.00904

D39 1.02005 -0.00001 0.00000 -0.00280 -0.00274 1.01731

D40 1.02529 -0.00001 0.00000 -0.00374 -0.00380 1.02149

D41 -3.12796 -0.00001 0.00000 -0.00668 -0.00672 -3.13468

D42 -1.10552 0.00000 0.00000 -0.00278 -0.00280 -1.10832

D43 -1.00431 -0.00001 0.00000 -0.00502 -0.00503 -1.00934

D44 1.12562 -0.00001 0.00000 -0.00796 -0.00795 1.11767

D45 -3.13513 0.00000 0.00000 -0.00406 -0.00403 -3.13916

D46 3.13696 -0.00001 0.00000 -0.00687 -0.00687 3.13008

D47 -1.05115 0.00000 0.00000 -0.00287 -0.00288 -1.05403

D48 1.04106 -0.00001 0.00000 -0.00746 -0.00748 1.03357

D49 1.01079 0.00000 0.00000 -0.00109 -0.00108 1.00970

D50 3.10586 0.00000 0.00000 0.00290 0.00291 3.10877

D51 -1.08511 0.00000 0.00000 -0.00168 -0.00169 -1.08681

D52 -1.01831 0.00000 0.00000 0.00031 0.00033 -1.01797

D53 1.07677 0.00000 0.00000 0.00431 0.00432 1.08110

D54 -3.11421 0.00000 0.00000 -0.00027 -0.00028 -3.11448

Item Value Threshold Converged?

Maximum Force 0.000215 0.000450 YES

RMS Force 0.000043 0.000300 YES

Maximum Displacement 0.578463 0.001800 NO

RMS Displacement 0.179750 0.001200 NO

Predicted change in Energy=-6.154688D-02

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:50:30 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.176564 -0.254857 -0.173034

2 6 0 -2.889992 0.086349 0.535097

3 8 0 -4.875064 0.608710 -0.737637

4 8 0 -4.396860 -1.655808 -0.210303

5 6 0 -2.486270 -0.918762 1.559973

6 16 0 -1.575570 0.253617 -0.863953

7 6 0 -0.035527 0.596791 -0.056104

8 16 0 1.169195 -0.728449 0.124636

9 16 0 0.257968 2.095192 0.756522

10 6 0 2.709752 0.256357 -0.027556

11 6 0 3.927692 -0.655282 -0.014891

12 6 0 5.268127 0.118481 -0.147374

13 6 0 6.481322 -0.826003 -0.139683

14 1 0 -3.019269 1.093052 0.936910

15 1 0 -5.212152 -1.876380 -0.722081

16 1 0 -1.561853 -0.592300 2.008904

17 1 0 -3.255978 -0.976353 2.336017

18 1 0 -2.335531 -1.936679 1.146279

19 1 0 2.618772 0.818875 -0.972429

20 1 0 2.757433 0.985049 0.805794

21 1 0 3.929678 -1.242162 0.925340

22 1 0 3.848036 -1.382516 -0.840748

23 1 0 5.256679 0.710586 -1.088804

24 1 0 5.364992 0.847309 0.671041

25 1 0 7.423093 -0.264342 -0.246040

26 1 0 6.541915 -1.407775 0.800347

27 1 0 6.418136 -1.544335 -0.966000

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.507694 0.000000

3 O 1.245964 2.415207 0.000000

4 O 1.418655 2.421029 2.373774 0.000000

5 C 2.510216 1.491178 3.649455 2.706931 0.000000

6 S 2.738811 1.926921 3.320949 3.468838 2.842405

7 C 4.229322 2.959398 4.887304 4.911130 3.303747

8 S 5.374946 4.160453 6.250166 5.652712 3.931772

9 S 5.104104 3.740873 5.548887 6.055756 4.154551

10 C 6.906798 5.630507 7.626126 7.361637 5.558758

11 C 8.115684 6.879921 8.922362 8.386740 6.609730

12 C 9.452103 8.186679 10.172171 9.826701 8.007595

13 C 10.673231 9.439768 11.462261 10.910014 9.127712

14 H 2.094795 1.091612 2.546108 3.281781 2.172486

15 H 2.000808 3.290171 2.507897 0.987557 3.681744

16 H 3.422198 2.096813 4.468029 3.754091 1.078268

17 H 2.768280 2.122874 3.818536 2.871762 1.094537

18 H 2.821084 2.184860 4.059233 2.483603 1.109063

19 H 6.925932 5.758099 7.500458 7.478234 5.957676

20 H 7.111666 5.724888 7.796077 7.693536 5.629360

21 H 8.239682 6.958816 9.149574 8.413800 6.455365

22 H 8.130908 7.032178 8.948077 8.273479 6.789842

23 H 9.526636 8.330365 10.138339 9.978097 8.344103

24 H 9.642019 8.291097 10.339247 10.116132 8.096389

25 H 11.599891 10.348569 12.338903 11.901628 10.093830

26 H 10.824163 9.553200 11.695256 10.988164 9.073273

27 H 10.702300 9.568368 11.498875 10.841940 9.276870

6 7 8 9 10

6 S 0.000000

7 C 1.772603 0.000000

8 S 3.078230 1.800079 0.000000

9 S 3.062549 1.729656 3.033573 0.000000

10 C 4.366183 2.766454 1.834753 3.163438 0.000000

11 C 5.642066 4.156500 2.762993 4.650491 1.521389

12 C 6.882438 5.325961 4.194345 5.461329 2.564888

13 C 8.161106 6.670881 5.319593 6.933015 3.925406

14 H 2.456018 3.183562 4.639061 3.431779 5.869577

15 H 4.216840 5.775599 6.538827 6.919672 8.233316

16 H 2.994841 2.829818 3.320787 3.478911 4.807702

17 H 3.817906 4.309098 4.953162 4.927170 6.534216

18 H 3.068545 3.626874 3.845345 4.809796 5.625138

19 H 4.233650 2.816785 2.387266 3.192437 1.103400

20 H 4.700848 2.948600 2.433630 2.735356 1.108034

21 H 5.978853 4.479714 2.919811 4.964664 2.154481

22 H 5.665066 4.428926 2.921636 5.247315 2.154733

23 H 6.851206 5.393225 4.500088 5.505405 2.796321

24 H 7.133028 5.455007 4.515117 5.257967 2.808480

25 H 9.034713 7.510569 6.282041 7.609964 4.747046

26 H 8.451254 6.929253 5.457490 7.194491 4.259135

27 H 8.194046 6.860183 5.422780 7.359410 4.227917

11 12 13 14 15

11 C 0.000000

12 C 1.553392 0.000000

13 C 2.562370 1.537514 0.000000

14 H 7.226539 8.414654 9.752079 0.000000

15 H 9.248132 10.683914 11.754990 4.047037 0.000000

16 H 5.851053 7.197456 8.328487 2.472579 4.736224

17 H 7.565379 8.945740 10.048218 2.509177 3.740137

18 H 6.497558 7.982033 8.979098 3.112974 3.430648

19 H 2.191642 2.861879 4.279998 5.958880 8.285556

20 H 2.175711 2.821889 4.247492 5.779199 8.604444

21 H 1.108362 2.189409 2.796131 7.330841 9.310708

22 H 1.103292 2.179546 2.781257 7.513214 9.074414

23 H 2.187485 1.112209 2.182128 8.528840 10.789963

24 H 2.189546 1.100171 2.168742 8.392074 11.010687

25 H 3.524782 2.190928 1.101684 10.596453 12.746556

26 H 2.839898 2.202309 1.107153 9.883776 11.861512

27 H 2.810220 2.181199 1.096719 9.982059 11.637583

16 17 18 19 20

16 H 0.000000

17 H 1.767642 0.000000

18 H 1.774840 1.784636 0.000000

19 H 5.325166 6.977202 6.052035 0.000000

20 H 4.753076 6.507671 5.881387 1.791346 0.000000

21 H 5.635011 7.327640 6.307457 3.093199 2.519707

22 H 6.165375 7.792548 6.518579 2.524788 3.083161

23 H 7.601690 9.329549 8.345374 2.642693 3.148185

24 H 7.200245 8.967664 8.202104 3.200551 2.614669

25 H 9.269390 11.009838 9.998300 4.978202 4.943250

26 H 8.233873 9.926888 8.899914 4.846830 4.477493

27 H 8.569519 10.237890 9.013454 4.474368 4.789341

21 22 23 24 25

21 H 0.000000

22 H 1.773536 0.000000

23 H 3.103374 2.535130 0.000000

24 H 2.547682 3.091728 1.768467 0.000000

25 H 3.812114 3.792759 2.520731 2.512486 0.000000

26 H 2.620465 3.154491 3.115794 2.547013 1.782929

27 H 3.140207 2.578234 2.539435 3.083663 1.779512

26 27

26 H 0.000000

27 H 1.775937 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 7.91D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.217190 -0.288853 -0.175254

2 6 0 -2.927495 0.128311 0.484898

3 8 0 -4.919132 0.507404 -0.827694

4 8 0 -4.436493 -1.685513 -0.057645

5 6 0 -2.517983 -0.758269 1.611790

6 16 0 -1.619992 0.141596 -0.930477

7 6 0 -0.076350 0.571725 -0.172666

8 16 0 1.130340 -0.725351 0.146359

9 16 0 0.219818 2.150268 0.469358

10 6 0 2.669319 0.237298 -0.120413

11 6 0 3.888068 -0.667091 -0.013853

12 6 0 5.227200 0.087888 -0.236921

13 6 0 6.441206 -0.849695 -0.131681

14 1 0 -3.055670 1.172957 0.774560

15 1 0 -5.254064 -1.961104 -0.538160

16 1 0 -1.591681 -0.384282 2.017696

17 1 0 -3.283883 -0.730670 2.393230

18 1 0 -2.368396 -1.815356 1.311442

19 1 0 2.573303 0.692818 -1.120800

20 1 0 2.720419 1.052969 0.627790

21 1 0 3.895089 -1.147361 0.985025

22 1 0 3.805028 -1.480500 -0.754612

23 1 0 5.210706 0.573217 -1.237518

24 1 0 5.327410 0.902072 0.496181

25 1 0 7.381982 -0.302796 -0.303577

26 1 0 6.506830 -1.324892 0.866151

27 1 0 6.374627 -1.654302 -0.873953

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3932457 0.1867635 0.1762968

Leave Link 202 at Sat Aug 17 17:50:30 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1092.4686598682 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0543134114 Hartrees.

Nuclear repulsion after empirical dispersion term = 1092.4143464568 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2326

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.21D-08

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 93

GePol: Fraction of low-weight points (<1% of avg) = 4.00%

GePol: Cavity surface area = 313.017 Ang\*\*2

GePol: Cavity volume = 322.953 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0055639976 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1092.4087824592 Hartrees.

Leave Link 301 at Sat Aug 17 17:50:30 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.91D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:50:30 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:50:30 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999317 -0.036354 0.001139 0.006465 Ang= -4.23 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7553 S= 0.5027

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.60971545132

Leave Link 401 at Sat Aug 17 17:50:31 2019, MaxMem= 1342177280 cpu: 7.5

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16230828.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.66D-15 for 2296.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.20D-15 for 2297 1815.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.44D-15 for 2296.

Iteration 1 A^-1\*A deviation from orthogonality is 7.75D-10 for 815 813.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.44D-15 for 744.

Iteration 2 A\*A^-1 deviation from orthogonality is 3.08D-15 for 987 74.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 2130.

Iteration 2 A^-1\*A deviation from orthogonality is 3.58D-16 for 2314 2226.

E= -1658.60906213921

DIIS: error= 7.39D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.60906213921 IErMin= 1 ErrMin= 7.39D-03

ErrMax= 7.39D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.24D-01 BMatP= 1.24D-01

IDIUse=3 WtCom= 9.26D-01 WtEn= 7.39D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.432 Goal= None Shift= 0.000

Gap= 0.482 Goal= None Shift= 0.000

GapD= 0.432 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=8.33D-04 MaxDP=1.97D-02 OVMax= 4.65D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 8.33D-04 CP: 9.99D-01

E= -1658.66196514300 Delta-E= -0.052903003794 Rises=F Damp=F

DIIS: error= 1.13D-03 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.66196514300 IErMin= 2 ErrMin= 1.13D-03

ErrMax= 1.13D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.36D-03 BMatP= 1.24D-01

IDIUse=3 WtCom= 9.89D-01 WtEn= 1.13D-02

Coeff-Com: -0.890D-02 0.101D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.880D-02 0.101D+01

Gap= 0.107 Goal= None Shift= 0.000

Gap= 0.123 Goal= None Shift= 0.000

RMSDP=2.14D-04 MaxDP=8.22D-03 DE=-5.29D-02 OVMax= 1.69D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.13D-04 CP: 9.99D-01 1.03D+00

E= -1658.66208382367 Delta-E= -0.000118680666 Rises=F Damp=F

DIIS: error= 1.25D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.66208382367 IErMin= 2 ErrMin= 1.13D-03

ErrMax= 1.25D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.04D-03 BMatP= 4.36D-03

IDIUse=3 WtCom= 2.21D-01 WtEn= 7.79D-01

Coeff-Com: -0.341D-01 0.542D+00 0.492D+00

Coeff-En: 0.000D+00 0.470D+00 0.530D+00

Coeff: -0.753D-02 0.486D+00 0.522D+00

Gap= 0.109 Goal= None Shift= 0.000

Gap= 0.125 Goal= None Shift= 0.000

RMSDP=1.45D-04 MaxDP=6.31D-03 DE=-1.19D-04 OVMax= 1.32D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 8.47D-05 CP: 9.99D-01 1.08D+00 4.77D-01

E= -1658.66306910137 Delta-E= -0.000985277701 Rises=F Damp=F

DIIS: error= 6.67D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.66306910137 IErMin= 4 ErrMin= 6.67D-04

ErrMax= 6.67D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.84D-04 BMatP= 4.36D-03

IDIUse=3 WtCom= 9.93D-01 WtEn= 6.67D-03

Coeff-Com: -0.197D-01 0.241D+00 0.338D+00 0.440D+00

Coeff-En: 0.000D+00 0.000D+00 0.129D+00 0.871D+00

Coeff: -0.196D-01 0.240D+00 0.337D+00 0.443D+00

Gap= 0.110 Goal= None Shift= 0.000

Gap= 0.125 Goal= None Shift= 0.000

RMSDP=5.36D-05 MaxDP=2.67D-03 DE=-9.85D-04 OVMax= 5.70D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.06D-05 CP: 9.99D-01 1.07D+00 6.06D-01 5.94D-01

E= -1658.66326548809 Delta-E= -0.000196386718 Rises=F Damp=F

DIIS: error= 2.05D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.66326548809 IErMin= 5 ErrMin= 2.05D-04

ErrMax= 2.05D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.56D-05 BMatP= 8.84D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.05D-03

Coeff-Com: -0.551D-02 0.524D-01 0.119D+00 0.269D+00 0.565D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.122D-01 0.988D+00

Coeff: -0.550D-02 0.523D-01 0.119D+00 0.268D+00 0.566D+00

Gap= 0.109 Goal= None Shift= 0.000

Gap= 0.125 Goal= None Shift= 0.000

RMSDP=1.71D-05 MaxDP=5.61D-04 DE=-1.96D-04 OVMax= 2.44D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.19D-05 CP: 9.99D-01 1.08D+00 6.08D-01 7.07D-01 7.94D-01

E= -1658.66328137244 Delta-E= -0.000015884350 Rises=F Damp=F

DIIS: error= 7.49D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.66328137244 IErMin= 6 ErrMin= 7.49D-05

ErrMax= 7.49D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.89D-06 BMatP= 6.56D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.245D-03-0.481D-02 0.143D-01 0.691D-01 0.269D+00 0.652D+00

Coeff: -0.245D-03-0.481D-02 0.143D-01 0.691D-01 0.269D+00 0.652D+00

Gap= 0.109 Goal= None Shift= 0.000

Gap= 0.125 Goal= None Shift= 0.000

RMSDP=6.77D-06 MaxDP=2.20D-04 DE=-1.59D-05 OVMax= 1.04D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 4.39D-06 CP: 9.99D-01 1.08D+00 6.14D-01 7.60D-01 8.61D-01

CP: 9.67D-01

E= -1658.66328268384 Delta-E= -0.000001311399 Rises=F Damp=F

DIIS: error= 4.64D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.66328268384 IErMin= 7 ErrMin= 4.64D-05

ErrMax= 4.64D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.44D-06 BMatP= 4.89D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.811D-03-0.127D-01-0.129D-01-0.600D-02 0.719D-01 0.394D+00

Coeff-Com: 0.565D+00

Coeff: 0.811D-03-0.127D-01-0.129D-01-0.600D-02 0.719D-01 0.394D+00

Coeff: 0.565D+00

Gap= 0.109 Goal= None Shift= 0.000

Gap= 0.125 Goal= None Shift= 0.000

RMSDP=3.02D-06 MaxDP=1.22D-04 DE=-1.31D-06 OVMax= 2.80D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.20D-06 CP: 9.99D-01 1.08D+00 6.16D-01 7.68D-01 9.10D-01

CP: 1.06D+00 1.02D+00

E= -1658.66328307748 Delta-E= -0.000000393638 Rises=F Damp=F

DIIS: error= 2.43D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.66328307748 IErMin= 8 ErrMin= 2.43D-05

ErrMax= 2.43D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.10D-07 BMatP= 1.44D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.526D-03-0.601D-02-0.114D-01-0.222D-01-0.260D-01 0.668D-01

Coeff-Com: 0.343D+00 0.656D+00

Coeff: 0.526D-03-0.601D-02-0.114D-01-0.222D-01-0.260D-01 0.668D-01

Coeff: 0.343D+00 0.656D+00

Gap= 0.109 Goal= None Shift= 0.000

Gap= 0.125 Goal= None Shift= 0.000

RMSDP=2.31D-06 MaxDP=9.18D-05 DE=-3.94D-07 OVMax= 3.63D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.05D-06 CP: 9.99D-01 1.08D+00 6.17D-01 7.83D-01 9.22D-01

CP: 1.16D+00 1.20D+00 9.39D-01

E= -1658.66328318966 Delta-E= -0.000000112187 Rises=F Damp=F

DIIS: error= 8.14D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.66328318966 IErMin= 9 ErrMin= 8.14D-06

ErrMax= 8.14D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.69D-08 BMatP= 3.10D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.938D-04-0.183D-04-0.293D-02-0.105D-01-0.301D-01-0.563D-01

Coeff-Com: 0.335D-01 0.369D+00 0.697D+00

Coeff: 0.938D-04-0.183D-04-0.293D-02-0.105D-01-0.301D-01-0.563D-01

Coeff: 0.335D-01 0.369D+00 0.697D+00

Gap= 0.109 Goal= None Shift= 0.000

Gap= 0.125 Goal= None Shift= 0.000

RMSDP=1.07D-06 MaxDP=4.75D-05 DE=-1.12D-07 OVMax= 1.70D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 3.98D-07 CP: 9.99D-01 1.08D+00 6.17D-01 7.89D-01 9.31D-01

CP: 1.20D+00 1.34D+00 1.09D+00 8.70D-01

E= -1658.66328321721 Delta-E= -0.000000027545 Rises=F Damp=F

DIIS: error= 1.82D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.66328321721 IErMin=10 ErrMin= 1.82D-06

ErrMax= 1.82D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.02D-08 BMatP= 6.69D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.464D-04 0.109D-02 0.495D-03-0.156D-02-0.112D-01-0.407D-01

Coeff-Com: -0.501D-01 0.623D-01 0.345D+00 0.695D+00

Coeff: -0.464D-04 0.109D-02 0.495D-03-0.156D-02-0.112D-01-0.407D-01

Coeff: -0.501D-01 0.623D-01 0.345D+00 0.695D+00

Gap= 0.109 Goal= None Shift= 0.000

Gap= 0.125 Goal= None Shift= 0.000

RMSDP=4.01D-07 MaxDP=2.01D-05 DE=-2.75D-08 OVMax= 4.98D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.76D-07 CP: 9.99D-01 1.08D+00 6.17D-01 7.91D-01 9.33D-01

CP: 1.21D+00 1.37D+00 1.16D+00 1.02D+00 8.42D-01

E= -1658.66328322136 Delta-E= -0.000000004150 Rises=F Damp=F

DIIS: error= 7.30D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.66328322136 IErMin=11 ErrMin= 7.30D-07

ErrMax= 7.30D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.04D-09 BMatP= 1.02D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.270D-04 0.402D-03 0.448D-03 0.491D-03-0.116D-02-0.840D-02

Coeff-Com: -0.225D-01-0.185D-01 0.648D-01 0.273D+00 0.711D+00

Coeff: -0.270D-04 0.402D-03 0.448D-03 0.491D-03-0.116D-02-0.840D-02

Coeff: -0.225D-01-0.185D-01 0.648D-01 0.273D+00 0.711D+00

Gap= 0.109 Goal= None Shift= 0.000

Gap= 0.125 Goal= None Shift= 0.000

RMSDP=1.19D-07 MaxDP=6.05D-06 DE=-4.15D-09 OVMax= 1.60D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 6.77D-08 CP: 9.99D-01 1.08D+00 6.17D-01 7.92D-01 9.33D-01

CP: 1.21D+00 1.38D+00 1.17D+00 1.05D+00 9.90D-01

CP: 1.05D+00

E= -1658.66328322184 Delta-E= -0.000000000477 Rises=F Damp=F

DIIS: error= 5.51D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.66328322184 IErMin=12 ErrMin= 5.51D-07

ErrMax= 5.51D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.36D-10 BMatP= 1.04D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.243D-06-0.103D-03 0.890D-04 0.702D-03 0.249D-02 0.713D-02

Coeff-Com: 0.274D-02-0.271D-01-0.586D-01-0.606D-01 0.355D+00 0.778D+00

Coeff: -0.243D-06-0.103D-03 0.890D-04 0.702D-03 0.249D-02 0.713D-02

Coeff: 0.274D-02-0.271D-01-0.586D-01-0.606D-01 0.355D+00 0.778D+00

Gap= 0.109 Goal= None Shift= 0.000

Gap= 0.125 Goal= None Shift= 0.000

RMSDP=6.51D-08 MaxDP=2.80D-06 DE=-4.77D-10 OVMax= 7.36D-06

Cycle 13 Pass 1 IDiag 1:

RMSU= 2.81D-08 CP: 9.99D-01 1.08D+00 6.17D-01 7.92D-01 9.32D-01

CP: 1.21D+00 1.38D+00 1.17D+00 1.07D+00 1.05D+00

CP: 1.28D+00 1.09D+00

E= -1658.66328322198 Delta-E= -0.000000000141 Rises=F Damp=F

DIIS: error= 2.51D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1658.66328322198 IErMin=13 ErrMin= 2.51D-07

ErrMax= 2.51D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.38D-11 BMatP= 3.36D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.482D-05-0.129D-03-0.420D-04 0.258D-03 0.155D-02 0.541D-02

Coeff-Com: 0.606D-02-0.975D-02-0.422D-01-0.956D-01 0.311D-01 0.410D+00

Coeff-Com: 0.694D+00

Coeff: 0.482D-05-0.129D-03-0.420D-04 0.258D-03 0.155D-02 0.541D-02

Coeff: 0.606D-02-0.975D-02-0.422D-01-0.956D-01 0.311D-01 0.410D+00

Coeff: 0.694D+00

Gap= 0.109 Goal= None Shift= 0.000

Gap= 0.125 Goal= None Shift= 0.000

RMSDP=2.70D-08 MaxDP=1.24D-06 DE=-1.41D-10 OVMax= 2.55D-06

Cycle 14 Pass 1 IDiag 1:

RMSU= 1.51D-08 CP: 9.99D-01 1.08D+00 6.17D-01 7.92D-01 9.32D-01

CP: 1.21D+00 1.38D+00 1.17D+00 1.07D+00 1.07D+00

CP: 1.38D+00 1.22D+00 9.65D-01

E= -1658.66328322198 Delta-E= -0.000000000008 Rises=F Damp=F

DIIS: error= 1.14D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1658.66328322198 IErMin=14 ErrMin= 1.14D-07

ErrMax= 1.14D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.12D-11 BMatP= 7.38D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.236D-05-0.407D-04-0.369D-04-0.180D-04 0.246D-03 0.106D-02

Coeff-Com: 0.226D-02 0.787D-03-0.767D-02-0.341D-01-0.535D-01 0.425D-01

Coeff-Com: 0.326D+00 0.722D+00

Coeff: 0.236D-05-0.407D-04-0.369D-04-0.180D-04 0.246D-03 0.106D-02

Coeff: 0.226D-02 0.787D-03-0.767D-02-0.341D-01-0.535D-01 0.425D-01

Coeff: 0.326D+00 0.722D+00

Gap= 0.109 Goal= None Shift= 0.000

Gap= 0.125 Goal= None Shift= 0.000

RMSDP=9.92D-09 MaxDP=4.40D-07 DE=-8.19D-12 OVMax= 1.08D-06

Error on total polarization charges = 0.04165

SCF Done: E(UB3LYP) = -1658.66328322 A.U. after 14 cycles

NFock= 14 Conv=0.99D-08 -V/T= 2.0024

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7553 S= 0.5027

<L.S>= 0.000000000000E+00

KE= 1.654759147800D+03 PE=-6.127309729514D+03 EE= 1.721478516033D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.49

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7553, after 0.7500

Leave Link 502 at Sat Aug 17 17:51:01 2019, MaxMem= 1342177280 cpu: 347.4

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 337

Leave Link 701 at Sat Aug 17 17:51:02 2019, MaxMem= 1342177280 cpu: 10.3

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:51:02 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:51:05 2019, MaxMem= 1342177280 cpu: 36.5

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.15323367D+00-2.79730315D+00 4.27502928D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.018406751 0.010684278 -0.028965125

2 6 -0.012037358 -0.001894553 -0.011721774

3 8 0.021873844 -0.050491078 0.023991591

4 8 -0.009515631 0.036618144 -0.006512101

5 6 0.002796595 -0.013894023 0.004656897

6 16 0.009826945 -0.002866499 0.001101457

7 6 -0.006796731 0.006432645 0.004984950

8 16 -0.006845698 -0.000066285 -0.002686259

9 16 -0.007635650 0.001337968 -0.001176412

10 6 0.004521768 0.008891926 0.001803433

11 6 0.006725338 -0.002918594 -0.000015989

12 6 -0.004960012 -0.001887348 -0.003566899

13 6 -0.000402020 0.001059431 0.003148147

14 1 0.002634541 -0.002222165 0.001204294

15 1 0.011053906 0.010324070 0.006270668

16 1 0.007862401 0.000118466 0.007131352

17 1 0.001670707 -0.001087680 0.001938503

18 1 -0.001899289 0.012183369 0.002542017

19 1 0.003295876 -0.002887549 0.006281244

20 1 -0.002106927 -0.008275816 -0.009135748

21 1 0.001585093 0.003702249 -0.006245623

22 1 0.001844192 0.002433580 0.003615148

23 1 0.000098137 -0.005748259 0.007921146

24 1 -0.001523261 -0.002234702 -0.001616353

25 1 -0.003869917 -0.002994953 0.000316842

26 1 -0.000919653 0.004667794 -0.006141783

27 1 0.001129556 0.001015582 0.000876377

-------------------------------------------------------------------

Cartesian Forces: Max 0.050491078 RMS 0.010223688

Leave Link 716 at Sat Aug 17 17:51:05 2019, MaxMem= 1342177280 cpu: 0.3

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.058137433 RMS 0.009133702

Search for a local minimum.

Step number 45 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .91337D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43 45 44

ITU= 0 1 1 1 1 1 -1 -1 0 -1 -1 -1 0 -1 0 0 -1 -1 0 0

ITU= -1 0 0 -1 1 -1 1 -1 1 1 -1 1 -1 1 1 -1 0 0 -1 0

ITU= 0 -1 -1 0 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.99457.

Iteration 1 RMS(Cart)= 0.17810864 RMS(Int)= 0.00766187

Iteration 2 RMS(Cart)= 0.01374824 RMS(Int)= 0.00003050

Iteration 3 RMS(Cart)= 0.00008294 RMS(Int)= 0.00000177

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000177

ITry= 1 IFail=0 DXMaxC= 5.75D-01 DCOld= 1.00D+10 DXMaxT= 1.20D-01 DXLimC= 3.00D+00 Rises=T

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.84913 -0.00343 -0.01370 0.00000 -0.01370 2.83543

R2 2.35453 -0.05814 -0.06481 0.00000 -0.06481 2.28972

R3 2.68087 -0.04656 -0.12746 0.00000 -0.12746 2.55341

R4 2.81792 0.01580 0.04718 0.00000 0.04718 2.86510

R5 3.64135 -0.00374 -0.03060 0.00000 -0.03060 3.61075

R6 2.06285 -0.00192 -0.00469 0.00000 -0.00469 2.05815

R7 1.86621 -0.01469 -0.02916 0.00000 -0.02916 1.83705

R8 2.03763 0.00975 0.02359 0.00000 0.02359 2.06122

R9 2.06837 0.00026 0.00024 0.00000 0.00024 2.06862

R10 2.09582 -0.01240 -0.03570 0.00000 -0.03570 2.06012

R11 3.34973 -0.01404 -0.03455 0.00000 -0.03455 3.31519

R12 3.40166 0.00234 -0.01400 0.00000 -0.01400 3.38766

R13 3.26858 -0.00070 -0.01480 0.00000 -0.01480 3.25378

R14 3.46718 0.00202 0.00503 0.00000 0.00503 3.47221

R15 2.87501 0.00148 0.00636 0.00000 0.00636 2.88137

R16 2.08512 -0.00712 -0.02083 0.00000 -0.02083 2.06430

R17 2.09388 -0.01241 -0.03375 0.00000 -0.03375 2.06013

R18 2.93549 -0.01213 -0.04127 0.00000 -0.04127 2.89421

R19 2.09450 -0.00725 -0.02227 0.00000 -0.02227 2.07223

R20 2.08492 -0.00445 -0.01375 0.00000 -0.01375 2.07117

R21 2.90548 -0.00552 -0.01928 0.00000 -0.01928 2.88620

R22 2.10177 -0.00976 -0.02979 0.00000 -0.02979 2.07198

R23 2.07902 -0.00282 -0.00720 0.00000 -0.00720 2.07182

R24 2.08188 -0.00486 -0.01421 0.00000 -0.01421 2.06768

R25 2.09222 -0.00771 -0.02294 0.00000 -0.02294 2.06928

R26 2.07250 -0.00140 -0.00343 0.00000 -0.00343 2.06907

A1 2.13456 0.01375 0.04156 0.00000 0.04156 2.17612

A2 1.94801 0.00763 0.02946 0.00000 0.02946 1.97748

A3 2.19627 -0.02108 -0.06724 0.00000 -0.06724 2.12903

A4 1.98373 0.01083 0.04397 0.00000 0.04397 2.02770

A5 1.83457 -0.00530 -0.00556 0.00000 -0.00556 1.82901

A6 1.85514 -0.00128 0.01898 0.00000 0.01898 1.87412

A7 1.95287 -0.00140 -0.00597 0.00000 -0.00597 1.94690

A8 1.98306 -0.00514 -0.04208 0.00000 -0.04207 1.94099

A9 1.84210 0.00171 -0.01056 0.00000 -0.01056 1.83154

A10 1.94161 -0.01348 -0.06957 0.00000 -0.06957 1.87204

A11 1.89039 0.00592 0.02245 0.00000 0.02245 1.91285

A12 1.90962 0.00355 0.01679 0.00000 0.01679 1.92641

A13 1.98130 -0.00497 -0.02889 0.00000 -0.02889 1.95241

A14 1.90035 -0.00395 -0.01694 0.00000 -0.01694 1.88342

A15 1.89301 -0.00088 0.00135 0.00000 0.00135 1.89435

A16 1.88784 0.00018 0.00495 0.00000 0.00495 1.89279

A17 1.85308 -0.01569 -0.05415 0.00000 -0.05415 1.79893

A18 2.07680 -0.02270 -0.10697 0.00000 -0.10697 1.96983

A19 2.12852 -0.00127 0.01429 0.00000 0.01429 2.14281

A20 2.06809 0.02333 0.08716 0.00000 0.08716 2.15525

A21 1.72992 0.02570 0.06556 0.00000 0.06556 1.79548

A22 1.92822 -0.00059 -0.00149 0.00000 -0.00149 1.92673

A23 1.84984 0.00274 0.02948 0.00000 0.02948 1.87932

A24 1.90365 -0.00160 -0.01170 0.00000 -0.01170 1.89195

A25 1.95910 -0.00269 -0.01999 0.00000 -0.01999 1.93911

A26 1.93196 0.00229 0.00616 0.00000 0.00616 1.93812

A27 1.88843 -0.00015 -0.00170 0.00000 -0.00170 1.88673

A28 1.97318 -0.00327 -0.02044 0.00000 -0.02044 1.95273

A29 1.90264 0.00200 0.01350 0.00000 0.01350 1.91614

A30 1.90810 0.00195 0.00907 0.00000 0.00907 1.91717

A31 1.91193 -0.00013 -0.00503 0.00000 -0.00503 1.90690

A32 1.90370 0.00024 0.00482 0.00000 0.00482 1.90853

A33 1.86095 -0.00065 -0.00093 0.00000 -0.00093 1.86002

A34 1.95463 0.00157 0.01157 0.00000 0.01157 1.96619

A35 1.90550 -0.00030 0.00070 0.00000 0.00070 1.90620

A36 1.92039 -0.00154 -0.01268 0.00000 -0.01268 1.90771

A37 1.91706 -0.00090 -0.00417 0.00000 -0.00417 1.91289

A38 1.91108 0.00051 0.00166 0.00000 0.00166 1.91274

A39 1.85241 0.00058 0.00235 0.00000 0.00235 1.85476

A40 1.93999 0.00074 0.00545 0.00000 0.00545 1.94545

A41 1.95004 -0.00153 -0.00793 0.00000 -0.00793 1.94211

A42 1.93170 0.00133 0.01123 0.00000 0.01123 1.94293

A43 1.87872 0.00013 -0.00180 0.00000 -0.00180 1.87691

A44 1.88645 -0.00102 -0.00935 0.00000 -0.00935 1.87710

A45 1.87412 0.00030 0.00183 0.00000 0.00183 1.87595

D1 2.75119 -0.00157 -0.03223 0.00000 -0.03223 2.71897

D2 -1.39080 -0.00047 -0.01648 0.00000 -0.01648 -1.40728

D3 0.55699 -0.00131 -0.02301 0.00000 -0.02300 0.53398

D4 -0.48501 0.00048 0.02704 0.00000 0.02703 -0.45798

D5 1.65618 0.00157 0.04279 0.00000 0.04278 1.69896

D6 -2.67921 0.00073 0.03626 0.00000 0.03625 -2.64296

D7 -3.08181 -0.00218 -0.01828 0.00000 -0.01829 -3.10010

D8 -0.03887 0.00232 0.04609 0.00000 0.04610 0.00722

D9 3.14078 -0.00124 -0.00164 0.00000 -0.00164 3.13915

D10 -1.07316 -0.00054 0.00114 0.00000 0.00113 -1.07203

D11 1.03734 -0.00109 -0.00014 0.00000 -0.00014 1.03720

D12 1.06612 -0.00094 -0.02144 0.00000 -0.02144 1.04468

D13 3.13536 -0.00024 -0.01867 0.00000 -0.01867 3.11670

D14 -1.03732 -0.00079 -0.01994 0.00000 -0.01994 -1.05726

D15 -1.01785 0.00149 0.02434 0.00000 0.02434 -0.99351

D16 1.05139 0.00220 0.02711 0.00000 0.02711 1.07851

D17 -3.12129 0.00165 0.02583 0.00000 0.02584 -3.09545

D18 -3.10621 -0.00319 0.01972 0.00000 0.01972 -3.08649

D19 -0.94526 0.00578 0.06669 0.00000 0.06669 -0.87857

D20 1.21991 -0.00028 0.00513 0.00000 0.00513 1.22504

D21 1.79248 -0.00186 0.03200 0.00000 0.03199 1.82447

D22 -1.19695 0.00113 0.06112 0.00000 0.06112 -1.13583

D23 2.55404 -0.00052 0.04095 0.00000 0.04095 2.59498

D24 -0.73442 -0.00539 0.00502 0.00000 0.00502 -0.72939

D25 -3.06595 0.00201 0.03978 0.00000 0.03978 -3.02617

D26 -0.93958 0.00011 0.03298 0.00000 0.03298 -0.90660

D27 1.08995 0.00059 0.04067 0.00000 0.04067 1.13062

D28 3.13699 0.00091 0.02272 0.00000 0.02272 -3.12347

D29 -1.01534 -0.00002 0.01213 0.00000 0.01213 -1.00321

D30 1.01275 0.00140 0.02394 0.00000 0.02394 1.03669

D31 1.07641 -0.00042 -0.00040 0.00000 -0.00040 1.07600

D32 -3.07593 -0.00135 -0.01099 0.00000 -0.01099 -3.08692

D33 -1.04784 0.00008 0.00082 0.00000 0.00081 -1.04703

D34 -1.03567 0.00002 0.01110 0.00000 0.01110 -1.02457

D35 1.09518 -0.00091 0.00050 0.00000 0.00050 1.09568

D36 3.12327 0.00051 0.01231 0.00000 0.01231 3.13558

D37 -3.13606 0.00031 0.00372 0.00000 0.00372 -3.13234

D38 -1.00904 0.00001 0.00662 0.00000 0.00662 -1.00242

D39 1.01731 -0.00033 0.00273 0.00000 0.00273 1.02004

D40 1.02149 0.00008 0.00378 0.00000 0.00378 1.02527

D41 -3.13468 -0.00022 0.00668 0.00000 0.00668 -3.12799

D42 -1.10832 -0.00056 0.00279 0.00000 0.00279 -1.10553

D43 -1.00934 0.00079 0.00500 0.00000 0.00500 -1.00434

D44 1.11767 0.00049 0.00790 0.00000 0.00790 1.12558

D45 -3.13916 0.00015 0.00401 0.00000 0.00401 -3.13515

D46 3.13008 0.00038 0.00683 0.00000 0.00683 3.13692

D47 -1.05403 0.00002 0.00287 0.00000 0.00287 -1.05117

D48 1.03357 0.00029 0.00744 0.00000 0.00744 1.04102

D49 1.00970 0.00033 0.00108 0.00000 0.00108 1.01078

D50 3.10877 -0.00004 -0.00289 0.00000 -0.00289 3.10588

D51 -1.08681 0.00023 0.00168 0.00000 0.00168 -1.08512

D52 -1.01797 -0.00015 -0.00033 0.00000 -0.00033 -1.01830

D53 1.08110 -0.00052 -0.00430 0.00000 -0.00430 1.07680

D54 -3.11448 -0.00025 0.00028 0.00000 0.00028 -3.11421

Item Value Threshold Converged?

Maximum Force 0.058137 0.000450 NO

RMS Force 0.009134 0.000300 NO

Maximum Displacement 0.575285 0.001800 NO

RMS Displacement 0.178772 0.001200 NO

Predicted change in Energy=-3.621948D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:51:05 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.094523 -0.408737 -0.207813

2 6 0 -2.845585 0.074740 0.468753

3 8 0 -4.886443 0.304283 -0.784533

4 8 0 -4.245710 -1.750432 -0.155290

5 6 0 -2.301462 -0.805558 1.576769

6 16 0 -1.577142 0.289271 -0.944015

7 6 0 -0.115829 0.762824 -0.096690

8 16 0 1.083327 -0.564679 0.019190

9 16 0 0.020688 2.244642 0.769486

10 6 0 2.687923 0.330316 0.000314

11 6 0 3.846751 -0.658009 -0.071875

12 6 0 5.203811 0.051899 -0.063736

13 6 0 6.377540 -0.921677 -0.148551

14 1 0 -3.039941 1.084613 0.827340

15 1 0 -5.054619 -1.969056 -0.648134

16 1 0 -1.396976 -0.356987 1.989594

17 1 0 -3.032725 -0.894859 2.386441

18 1 0 -2.059571 -1.806335 1.218429

19 1 0 2.685486 0.997423 -0.864702

20 1 0 2.751048 0.942605 0.900089

21 1 0 3.796378 -1.351690 0.775916

22 1 0 3.760725 -1.266639 -0.979302

23 1 0 5.248100 0.755461 -0.903515

24 1 0 5.291744 0.655261 0.847430

25 1 0 7.336209 -0.394278 -0.146072

26 1 0 6.380353 -1.615388 0.698689

27 1 0 6.332603 -1.520651 -1.063990

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.500446 0.000000

3 O 1.211668 2.405934 0.000000

4 O 1.351207 2.383492 2.242396 0.000000

5 C 2.560716 1.516145 3.672822 2.770002 0.000000

6 S 2.714114 1.910729 3.313175 3.450178 2.842119

7 C 4.149085 2.871367 4.841708 4.834853 3.168166

8 S 5.185169 4.005910 6.085985 5.462150 3.733747

9 S 4.993045 3.607552 5.500900 5.917599 3.917627

10 C 6.825767 5.559179 7.614964 7.240787 5.354380

11 C 7.946348 6.754004 8.814906 8.166288 6.367128

12 C 9.310852 8.067022 10.119114 9.620303 7.730175

13 C 10.484785 9.297309 11.348337 10.655530 8.849592

14 H 2.100900 1.089129 2.572279 3.233716 2.163271

15 H 1.884214 3.210043 2.283628 0.972125 3.726097

16 H 3.479660 2.144251 4.506599 3.828511 1.090749

17 H 2.844975 2.157005 3.863844 2.943422 1.094665

18 H 2.851048 2.172159 4.056817 2.582524 1.090171

19 H 6.955380 5.763870 7.604010 7.489689 5.837908

20 H 7.065084 5.679924 7.847080 7.571056 5.389046

21 H 8.007696 6.800347 8.976002 8.105635 6.174405

22 H 7.939528 6.894889 8.790861 8.063253 6.595165

23 H 9.440549 8.237368 10.145278 9.847424 8.098424

24 H 9.505137 8.166794 10.314164 9.887155 7.766769

25 H 11.430908 10.211117 12.259234 11.661049 9.799083

26 H 10.583042 9.382289 11.525006 10.661179 8.763604

27 H 10.521138 9.441065 11.369937 10.619757 9.057154

6 7 8 9 10

6 S 0.000000

7 C 1.754323 0.000000

8 S 2.955519 1.792671 0.000000

9 S 3.051659 1.721825 3.095873 0.000000

10 C 4.368550 2.838574 1.837417 3.372005 0.000000

11 C 5.574638 4.209683 2.766499 4.875657 1.524756

12 C 6.841971 5.367036 4.167185 5.689214 2.532057

13 C 8.085550 6.708508 5.308886 7.160862 3.899092

14 H 2.431059 3.083473 4.513824 3.273601 5.836211

15 H 4.156975 5.670882 6.331823 6.747121 8.102751

16 H 3.009348 2.692192 3.174513 3.204202 4.595218

17 H 3.822673 4.173983 4.759704 4.668441 6.318265

18 H 3.049667 3.479690 3.585762 4.575963 5.346754

19 H 4.321778 2.914146 2.405897 3.365602 1.092378

20 H 4.749821 3.040539 2.414369 3.027743 1.090173

21 H 5.875852 4.531884 2.924494 5.214353 2.158558

22 H 5.560119 4.463788 2.942481 5.419893 2.158893

23 H 6.841265 5.424275 4.465365 5.687041 2.748119

24 H 7.108081 5.490426 4.459261 5.506018 2.757368

25 H 8.975064 7.541498 6.257386 7.830645 4.706700

26 H 8.345534 6.963398 5.442811 7.439771 4.231729

27 H 8.115065 6.908850 5.444452 7.574915 4.224040

11 12 13 14 15

11 C 0.000000

12 C 1.531551 0.000000

13 C 2.545642 1.527312 0.000000

14 H 7.160436 8.355834 9.678146 0.000000

15 H 9.015837 10.471923 11.490903 3.944724 0.000000

16 H 5.642424 6.924864 8.082923 2.475557 4.789022

17 H 7.309351 8.645244 9.745768 2.519753 3.801395

18 H 6.153712 7.606162 8.592793 3.077605 3.532825

19 H 2.171996 2.806693 4.222212 5.970856 8.291932

20 H 2.169619 2.781792 4.210301 5.793187 8.473677

21 H 1.096576 2.157763 2.775238 7.257649 8.986057

22 H 1.096018 2.158541 2.767104 7.418989 8.849484

23 H 2.157152 1.096445 2.158332 8.473241 10.659936

24 H 2.158195 1.096359 2.158162 8.342764 10.778265

25 H 3.500196 2.180131 1.094167 10.526117 12.500585

26 H 2.815933 2.178391 1.095015 9.800434 11.519445

27 H 2.812099 2.178897 1.094905 9.910051 11.403633

16 17 18 19 20

16 H 0.000000

17 H 1.767051 0.000000

18 H 1.770406 1.772589 0.000000

19 H 5.162163 6.844604 5.892033 0.000000

20 H 4.481301 6.248003 5.549780 1.766860 0.000000

21 H 5.425254 7.031297 5.890217 3.073115 2.524266

22 H 6.020273 7.590613 6.244769 2.509033 3.071208

23 H 7.332439 9.061977 8.029165 2.574304 3.085982

24 H 6.860624 8.606289 7.761374 3.137045 2.557435

25 H 8.990605 10.685457 9.598773 4.907391 4.889316

26 H 7.983537 9.590293 8.458068 4.787798 4.444744

27 H 8.391953 10.000323 8.701703 4.436426 4.769987

21 22 23 24 25

21 H 0.000000

22 H 1.757638 0.000000

23 H 3.060730 2.511358 0.000000

24 H 2.503814 3.061808 1.754353 0.000000

25 H 3.781150 3.773509 2.501164 2.503681 0.000000

26 H 2.598544 3.130452 3.077333 2.522507 1.765896

27 H 3.137871 2.585778 2.526378 3.077581 1.765931

26 27

26 H 0.000000

27 H 1.765868 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 7.86D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.103841 -0.464044 -0.131068

2 6 0 -2.849362 0.121862 0.447149

3 8 0 -4.899840 0.145813 -0.811215

4 8 0 -4.255389 -1.778516 0.142712

5 6 0 -2.297087 -0.565093 1.680753

6 16 0 -1.591900 0.098602 -0.991299

7 6 0 -0.123721 0.702426 -0.244643

8 16 0 1.075537 -0.590134 0.078988

9 16 0 0.020435 2.306333 0.364770

10 6 0 2.680454 0.286564 -0.099176

11 6 0 3.838108 -0.702321 -0.016558

12 6 0 5.195602 -0.003279 -0.135725

13 6 0 6.368066 -0.979720 -0.068103

14 1 0 -3.040318 1.177339 0.636110

15 1 0 -5.068261 -2.073763 -0.301242

16 1 0 -1.389136 -0.056382 2.007207

17 1 0 -3.022037 -0.518564 2.499638

18 1 0 -2.058590 -1.611646 1.490176

19 1 0 2.671628 0.802218 -1.062147

20 1 0 2.750980 1.038465 0.687048

21 1 0 3.793976 -1.246923 0.934199

22 1 0 3.744625 -1.451829 -0.810757

23 1 0 5.233719 0.552401 -1.080161

24 1 0 5.291018 0.741646 0.663014

25 1 0 7.327030 -0.460890 -0.159774

26 1 0 6.377113 -1.524542 0.881710

27 1 0 6.315613 -1.721100 -0.872106

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3053344 0.1933589 0.1808919

Leave Link 202 at Sat Aug 17 17:51:05 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.3347555415 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0550035446 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.2797519969 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2322

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.22D-09

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 95

GePol: Fraction of low-weight points (<1% of avg) = 4.09%

GePol: Cavity surface area = 309.114 Ang\*\*2

GePol: Cavity volume = 320.348 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057823247 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.2739696722 Hartrees.

Leave Link 301 at Sat Aug 17 17:51:05 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:51:05 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:51:05 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Lowest energy guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000185 0.000006 0.000038 Ang= -0.02 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999324 0.036167 -0.001133 -0.006428 Ang= 4.21 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 5.43D-03

Max alpha theta= 3.669 degrees.

Max beta theta= 4.074 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 17:51:06 2019, MaxMem= 1342177280 cpu: 4.3

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16175052.

Iteration 1 A\*A^-1 deviation from unit magnitude is 4.11D-15 for 2322.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.42D-15 for 775 110.

Iteration 1 A^-1\*A deviation from unit magnitude is 4.33D-15 for 2313.

Iteration 1 A^-1\*A deviation from orthogonality is 1.36D-11 for 773 715.

E= -1658.67701452443

DIIS: error= 5.65D-06 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67701452443 IErMin= 1 ErrMin= 5.65D-06

ErrMax= 5.65D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.30D-08 BMatP= 4.30D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 88.738 Goal= None Shift= 0.000

Gap= 88.673 Goal= None Shift= 0.000

RMSDP=5.30D-07 MaxDP=1.99D-05 OVMax= 2.74D-05

Cycle 2 Pass 1 IDiag 1:

RMSU= 5.29D-07 CP: 1.00D+00

E= -1658.67701453325 Delta-E= -0.000000008820 Rises=F Damp=F

DIIS: error= 5.21D-06 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67701453325 IErMin= 2 ErrMin= 5.21D-06

ErrMax= 5.21D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.97D-08 BMatP= 4.30D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.355D+00 0.645D+00

Coeff: 0.355D+00 0.645D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.00D-07 MaxDP=1.47D-05 DE=-8.82D-09 OVMax= 3.13D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.80D-07 CP: 1.00D+00 8.01D-01

E= -1658.67701453330 Delta-E= -0.000000000050 Rises=F Damp=F

DIIS: error= 5.93D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67701453330 IErMin= 2 ErrMin= 5.21D-06

ErrMax= 5.93D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.01D-08 BMatP= 1.97D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.887D-02 0.505D+00 0.504D+00

Coeff: -0.887D-02 0.505D+00 0.504D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.51D-07 MaxDP=7.17D-06 DE=-5.05D-11 OVMax= 1.75D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 4.50D-08 CP: 1.00D+00 9.19D-01 5.36D-01

E= -1658.67701453685 Delta-E= -0.000000003547 Rises=F Damp=F

DIIS: error= 6.81D-07 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67701453685 IErMin= 4 ErrMin= 6.81D-07

ErrMax= 6.81D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.60D-10 BMatP= 1.97D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.152D-01 0.256D+00 0.270D+00 0.489D+00

Coeff: -0.152D-01 0.256D+00 0.270D+00 0.489D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.57D-08 MaxDP=1.25D-06 DE=-3.55D-09 OVMax= 2.04D-06

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.67D-08 CP: 1.00D+00 9.28D-01 5.49D-01 5.86D-01

E= -1658.67701453691 Delta-E= -0.000000000057 Rises=F Damp=F

DIIS: error= 2.12D-07 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67701453691 IErMin= 5 ErrMin= 2.12D-07

ErrMax= 2.12D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.94D-11 BMatP= 3.60D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.562D-02 0.648D-01 0.695D-01 0.253D+00 0.619D+00

Coeff: -0.562D-02 0.648D-01 0.695D-01 0.253D+00 0.619D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.58D-09 MaxDP=3.81D-07 DE=-5.73D-11 OVMax= 4.96D-07

Error on total polarization charges = 0.04162

SCF Done: E(UB3LYP) = -1658.67701454 A.U. after 5 cycles

NFock= 5 Conv=0.66D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655234869534D+03 PE=-6.147313257288D+03 EE= 1.731127403545D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.63

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:51:19 2019, MaxMem= 1342177280 cpu: 144.2

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 337

Leave Link 701 at Sat Aug 17 17:51:20 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:51:20 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:51:23 2019, MaxMem= 1342177280 cpu: 38.6

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.40816587D+00-2.93984323D+00 6.43617840D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000237159 0.000112837 -0.000019112

2 6 0.000067780 0.000002090 0.000054321

3 8 0.000181144 -0.000153255 0.000129565

4 8 0.000004678 0.000115992 -0.000109668

5 6 -0.000022861 -0.000077475 -0.000023307

6 16 0.000048926 0.000049045 -0.000017165

7 6 -0.000069693 0.000003263 0.000050049

8 16 0.000021281 -0.000004735 -0.000023628

9 16 0.000004971 -0.000009196 0.000050297

10 6 0.000032822 0.000008742 0.000028419

11 6 0.000009275 0.000010819 -0.000004383

12 6 -0.000005874 0.000013331 -0.000008894

13 6 0.000012993 0.000002836 -0.000005098

14 1 -0.000047088 -0.000021211 0.000018630

15 1 0.000025162 0.000033671 -0.000005048

16 1 0.000021252 -0.000040832 0.000003786

17 1 0.000004038 -0.000052666 -0.000011815

18 1 0.000000523 -0.000012311 -0.000028208

19 1 -0.000004102 0.000008165 0.000026994

20 1 -0.000023883 -0.000021083 0.000016390

21 1 0.000002655 -0.000008404 -0.000037006

22 1 -0.000006999 0.000020926 -0.000017119

23 1 0.000001940 0.000009507 0.000021863

24 1 -0.000000227 -0.000014046 0.000009289

25 1 -0.000007610 0.000006141 -0.000014790

26 1 -0.000003172 -0.000010280 -0.000050005

27 1 -0.000010771 0.000028129 -0.000034354

-------------------------------------------------------------------

Cartesian Forces: Max 0.000237159 RMS 0.000052397

Leave Link 716 at Sat Aug 17 17:51:23 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000275911 RMS 0.000033092

Search for a local minimum.

Step number 46 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .33092D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43 45 44 46

ITU= 0 0 1 1 1 1 1 -1 -1 0 -1 -1 -1 0 -1 0 0 -1 -1 0

ITU= 0 -1 0 0 -1 1 -1 1 -1 1 1 -1 1 -1 1 1 -1 0 0 -1

ITU= 0 0 -1 -1 0 0

Use linear search instead of GDIIS.

Eigenvalues --- -0.02823 0.00000 0.00061 0.00152 0.00246

Eigenvalues --- 0.00317 0.00331 0.00515 0.00887 0.01235

Eigenvalues --- 0.02591 0.02873 0.03450 0.03619 0.03929

Eigenvalues --- 0.04608 0.04729 0.04812 0.05025 0.05444

Eigenvalues --- 0.05498 0.05543 0.05629 0.05877 0.07603

Eigenvalues --- 0.08184 0.08338 0.10906 0.11731 0.11987

Eigenvalues --- 0.13457 0.13817 0.14755 0.15758 0.15931

Eigenvalues --- 0.15997 0.16031 0.16162 0.16812 0.17864

Eigenvalues --- 0.18214 0.20436 0.21399 0.21836 0.22179

Eigenvalues --- 0.22893 0.23193 0.25041 0.25123 0.25646

Eigenvalues --- 0.27335 0.28931 0.29176 0.29472 0.29545

Eigenvalues --- 0.30764 0.32077 0.32727 0.33481 0.33855

Eigenvalues --- 0.33879 0.33918 0.33977 0.34007 0.34029

Eigenvalues --- 0.34075 0.34158 0.34225 0.34608 0.34738

Eigenvalues --- 0.35016 0.35443 0.47256 0.52166 0.82860

Eigenvalue 1 is -2.82D-02 should be greater than 0.000000 Eigenvector:

D26 D27 D25 D8 D23

1 -0.34428 -0.33191 -0.29193 -0.26956 -0.26878

D22 D19 D24 D5 D21

1 -0.24613 -0.23111 -0.20500 -0.18701 -0.18380

RFO step: Lambda=-2.82315523D-02 EMin=-2.82302439D-02

I= 1 Eig= -2.82D-02 Dot1= 5.75D-05

I= 1 Stepn= 2.99D-01 RXN= 2.99D-01 EDone=F

Mixed 1 eigenvectors in step. Raw Step.Grad= 5.75D-05.

RFO eigenvector is Hessian eigenvector with negative curvature.

Taking step of 2.99D-01 in eigenvector direction(s). Step.Grad= -1.20D-05.

Quartic linear search produced a step of -0.00784.

Iteration 1 RMS(Cart)= 0.13430300 RMS(Int)= 0.00749396

Iteration 2 RMS(Cart)= 0.01529784 RMS(Int)= 0.00017192

Iteration 3 RMS(Cart)= 0.00013483 RMS(Int)= 0.00016025

Iteration 4 RMS(Cart)= 0.00000002 RMS(Int)= 0.00016025

ITry= 1 IFail=0 DXMaxC= 3.89D-01 DCOld= 1.00D+10 DXMaxT= 1.20D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83543 -0.00001 0.00000 -0.00655 -0.00655 2.82889

R2 2.28972 -0.00028 0.00000 -0.02255 -0.02255 2.26717

R3 2.55341 -0.00012 -0.00001 -0.02237 -0.02238 2.53103

R4 2.86510 0.00001 0.00000 0.00668 0.00669 2.87178

R5 3.61075 0.00003 0.00000 -0.01136 -0.01137 3.59939

R6 2.05815 -0.00001 0.00000 -0.00218 -0.00218 2.05597

R7 1.83705 -0.00004 0.00000 -0.00814 -0.00814 1.82891

R8 2.06122 0.00002 0.00000 0.00129 0.00129 2.06251

R9 2.06862 0.00000 0.00000 -0.00083 -0.00083 2.06779

R10 2.06012 -0.00001 0.00000 -0.00468 -0.00468 2.05544

R11 3.31519 -0.00004 0.00000 0.01286 0.01285 3.32804

R12 3.38766 0.00003 0.00000 0.00601 0.00601 3.39367

R13 3.25378 0.00000 0.00000 0.00476 0.00476 3.25854

R14 3.47221 0.00000 0.00000 -0.00182 -0.00182 3.47039

R15 2.88137 0.00000 0.00000 -0.00044 -0.00044 2.88093

R16 2.06430 -0.00001 0.00000 -0.00233 -0.00233 2.06196

R17 2.06013 -0.00001 0.00000 -0.00462 -0.00462 2.05551

R18 2.89421 -0.00001 0.00000 -0.00220 -0.00220 2.89201

R19 2.07223 -0.00001 0.00000 -0.00199 -0.00199 2.07023

R20 2.07117 0.00000 0.00000 -0.00161 -0.00161 2.06956

R21 2.88620 -0.00001 0.00000 0.00236 0.00235 2.88856

R22 2.07198 -0.00001 0.00000 -0.00250 -0.00250 2.06948

R23 2.07182 0.00000 0.00000 -0.00292 -0.00292 2.06890

R24 2.06768 -0.00001 0.00000 -0.00232 -0.00232 2.06535

R25 2.06928 -0.00001 0.00000 -0.00269 -0.00269 2.06659

R26 2.06907 0.00000 0.00000 -0.00221 -0.00221 2.06687

A1 2.17612 0.00002 0.00000 0.01350 0.01283 2.18895

A2 1.97748 0.00000 0.00000 -0.01254 -0.01320 1.96428

A3 2.12903 -0.00002 0.00000 -0.00306 -0.00371 2.12532

A4 2.02770 0.00000 0.00000 -0.03046 -0.03035 1.99735

A5 1.82901 0.00001 0.00000 -0.00940 -0.00925 1.81977

A6 1.87412 -0.00004 0.00000 -0.01518 -0.01495 1.85917

A7 1.94690 -0.00003 0.00000 0.01842 0.01793 1.96483

A8 1.94099 0.00003 0.00000 0.02503 0.02449 1.96548

A9 1.83154 0.00002 0.00000 0.01311 0.01255 1.84408

A10 1.87204 0.00000 0.00000 0.01198 0.01198 1.88402

A11 1.91285 0.00000 0.00000 0.00488 0.00485 1.91769

A12 1.92641 0.00000 0.00000 -0.00697 -0.00695 1.91946

A13 1.95241 0.00000 0.00000 0.01175 0.01173 1.96414

A14 1.88342 0.00000 0.00000 -0.00143 -0.00142 1.88200

A15 1.89435 0.00000 0.00000 -0.00204 -0.00210 1.89225

A16 1.89279 0.00000 0.00000 -0.00667 -0.00664 1.88615

A17 1.79893 -0.00006 0.00000 -0.01035 -0.01035 1.78858

A18 1.96983 0.00004 0.00000 0.01029 0.01023 1.98006

A19 2.14281 -0.00002 0.00000 -0.00243 -0.00249 2.14032

A20 2.15525 -0.00002 0.00000 -0.00462 -0.00468 2.15057

A21 1.79548 0.00000 0.00000 0.00876 0.00877 1.80425

A22 1.92673 0.00001 0.00000 -0.01952 -0.01957 1.90716

A23 1.87932 -0.00002 0.00000 -0.01767 -0.01776 1.86156

A24 1.89195 -0.00001 0.00000 0.01062 0.01074 1.90269

A25 1.93911 0.00001 0.00000 0.00589 0.00560 1.94472

A26 1.93812 0.00000 0.00000 0.01398 0.01396 1.95208

A27 1.88673 0.00000 0.00000 0.00641 0.00631 1.89304

A28 1.95273 0.00000 0.00000 0.01691 0.01690 1.96963

A29 1.91614 -0.00001 0.00000 -0.00873 -0.00887 1.90727

A30 1.91717 0.00001 0.00000 -0.00793 -0.00796 1.90921

A31 1.90690 0.00001 0.00000 0.00750 0.00752 1.91442

A32 1.90853 -0.00001 0.00000 -0.00320 -0.00315 1.90537

A33 1.86002 0.00000 0.00000 -0.00558 -0.00564 1.85438

A34 1.96619 -0.00001 0.00000 -0.00883 -0.00883 1.95736

A35 1.90620 0.00000 0.00000 0.00015 0.00012 1.90632

A36 1.90771 0.00001 0.00000 0.00922 0.00922 1.91692

A37 1.91289 0.00000 0.00000 -0.00063 -0.00065 1.91224

A38 1.91274 0.00000 0.00000 -0.00022 -0.00019 1.91255

A39 1.85476 0.00000 0.00000 0.00091 0.00090 1.85566

A40 1.94545 0.00000 0.00000 -0.00040 -0.00040 1.94504

A41 1.94211 0.00000 0.00000 0.00516 0.00516 1.94727

A42 1.94293 -0.00001 0.00000 -0.00775 -0.00775 1.93519

A43 1.87691 0.00000 0.00000 0.00175 0.00174 1.87865

A44 1.87710 0.00001 0.00000 0.00460 0.00460 1.88170

A45 1.87595 0.00000 0.00000 -0.00318 -0.00317 1.87277

D1 2.71897 0.00002 0.00000 0.01394 0.01404 2.73301

D2 -1.40728 -0.00001 0.00000 0.01083 0.01106 -1.39622

D3 0.53398 0.00001 0.00000 0.01530 0.01519 0.54917

D4 -0.45798 -0.00002 0.00000 -0.05285 -0.05289 -0.51087

D5 1.69896 -0.00005 0.00000 -0.05595 -0.05587 1.64309

D6 -2.64296 -0.00003 0.00000 -0.05149 -0.05175 -2.69471

D7 -3.10010 0.00001 0.00000 -0.01629 -0.01659 -3.11669

D8 0.00722 -0.00003 0.00000 -0.08065 -0.08035 -0.07313

D9 3.13915 0.00000 0.00000 -0.00018 -0.00012 3.13902

D10 -1.07203 0.00001 0.00000 -0.00316 -0.00312 -1.07515

D11 1.03720 0.00001 0.00000 -0.00854 -0.00853 1.02867

D12 1.04468 0.00001 0.00000 0.02028 0.02052 1.06521

D13 3.11670 0.00001 0.00000 0.01730 0.01753 3.13422

D14 -1.05726 0.00001 0.00000 0.01192 0.01212 -1.04514

D15 -0.99351 -0.00002 0.00000 -0.02374 -0.02398 -1.01748

D16 1.07851 -0.00002 0.00000 -0.02672 -0.02697 1.05153

D17 -3.09545 -0.00002 0.00000 -0.03209 -0.03238 -3.12783

D18 -3.08649 -0.00003 0.00000 -0.03630 -0.03625 -3.12274

D19 -0.87857 -0.00004 0.00000 -0.06915 -0.06925 -0.94782

D20 1.22504 0.00000 0.00000 -0.02093 -0.02087 1.20416

D21 1.82447 -0.00007 0.00000 -0.05499 -0.05498 1.76950

D22 -1.13583 -0.00007 0.00000 -0.07364 -0.07365 -1.20948

D23 2.59498 -0.00002 0.00000 -0.08042 -0.08041 2.51457

D24 -0.72939 -0.00002 0.00000 -0.06133 -0.06134 -0.79073

D25 -3.02617 -0.00005 0.00000 -0.08734 -0.08751 -3.11368

D26 -0.90660 -0.00004 0.00000 -0.10301 -0.10280 -1.00940

D27 1.13062 -0.00005 0.00000 -0.09931 -0.09934 1.03128

D28 -3.12347 -0.00001 0.00000 -0.04265 -0.04261 3.11711

D29 -1.00321 -0.00001 0.00000 -0.02788 -0.02790 -1.03111

D30 1.03669 -0.00001 0.00000 -0.04443 -0.04436 0.99232

D31 1.07600 0.00000 0.00000 -0.01161 -0.01157 1.06444

D32 -3.08692 0.00000 0.00000 0.00316 0.00314 -3.08378

D33 -1.04703 0.00000 0.00000 -0.01339 -0.01332 -1.06035

D34 -1.02457 -0.00001 0.00000 -0.03308 -0.03313 -1.05771

D35 1.09568 -0.00001 0.00000 -0.01831 -0.01842 1.07726

D36 3.13558 -0.00001 0.00000 -0.03486 -0.03488 3.10070

D37 -3.13234 -0.00001 0.00000 -0.01155 -0.01153 3.13932

D38 -1.00242 -0.00001 0.00000 -0.01819 -0.01816 -1.02058

D39 1.02004 -0.00001 0.00000 -0.01188 -0.01183 1.00820

D40 1.02527 -0.00001 0.00000 -0.01685 -0.01690 1.00837

D41 -3.12799 -0.00001 0.00000 -0.02348 -0.02353 3.13166

D42 -1.10553 0.00000 0.00000 -0.01718 -0.01721 -1.12274

D43 -1.00434 0.00000 0.00000 -0.01258 -0.01258 -1.01692

D44 1.12558 0.00000 0.00000 -0.01922 -0.01921 1.10637

D45 -3.13515 0.00000 0.00000 -0.01291 -0.01289 3.13515

D46 3.13692 0.00000 0.00000 -0.00550 -0.00550 3.13142

D47 -1.05117 0.00000 0.00000 -0.00004 -0.00003 -1.05120

D48 1.04102 0.00000 0.00000 -0.00581 -0.00581 1.03521

D49 1.01078 0.00000 0.00000 0.00075 0.00074 1.01152

D50 3.10588 0.00000 0.00000 0.00621 0.00621 3.11209

D51 -1.08512 0.00000 0.00000 0.00044 0.00043 -1.08469

D52 -1.01830 0.00000 0.00000 0.00014 0.00014 -1.01816

D53 1.07680 0.00000 0.00000 0.00560 0.00561 1.08240

D54 -3.11421 0.00000 0.00000 -0.00017 -0.00017 -3.11438

Item Value Threshold Converged?

Maximum Force 0.000276 0.000450 YES

RMS Force 0.000033 0.000300 YES

Maximum Displacement 0.388543 0.001800 NO

RMS Displacement 0.144874 0.001200 NO

Predicted change in Energy=-1.320363D-03

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:51:23 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.073211 -0.371101 -0.172998

2 6 0 -2.817852 0.055652 0.521920

3 8 0 -4.869211 0.365910 -0.685407

4 8 0 -4.172776 -1.702317 -0.281851

5 6 0 -2.288546 -0.945705 1.535111

6 16 0 -1.586358 0.384226 -0.893495

7 6 0 -0.125582 0.849280 -0.026651

8 16 0 1.087892 -0.469598 0.087888

9 16 0 0.008819 2.334423 0.839176

10 6 0 2.691276 0.415303 -0.048753

11 6 0 3.830096 -0.597349 -0.006344

12 6 0 5.208489 0.052075 -0.149031

13 6 0 6.337983 -0.976732 -0.101199

14 1 0 -3.024010 1.028372 0.963509

15 1 0 -4.991405 -1.902202 -0.757837

16 1 0 -1.374873 -0.562595 1.992995

17 1 0 -3.024254 -1.096754 2.330882

18 1 0 -2.069952 -1.913601 1.089612

19 1 0 2.671650 0.953512 -0.997722

20 1 0 2.765148 1.141500 0.757678

21 1 0 3.781437 -1.157209 0.934058

22 1 0 3.693802 -1.331538 -0.807454

23 1 0 5.252249 0.600927 -1.095675

24 1 0 5.353625 0.793411 0.643417

25 1 0 7.315908 -0.501992 -0.214329

26 1 0 6.343051 -1.524509 0.845297

27 1 0 6.228765 -1.713025 -0.902577

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.496982 0.000000

3 O 1.199735 2.400411 0.000000

4 O 1.339365 2.360576 2.219334 0.000000

5 C 2.536304 1.519683 3.648406 2.724727 0.000000

6 S 2.697048 1.904715 3.289492 3.378953 2.856556

7 C 4.134552 2.859911 4.813483 4.791195 3.215507

8 S 5.168631 3.964733 6.064910 5.415804 3.704250

9 S 5.000733 3.644656 5.476730 5.919266 4.064659

10 C 6.811178 5.550271 7.587406 7.187062 5.399962

11 C 7.908301 6.700798 8.778778 8.083490 6.319432

12 C 9.291373 8.054337 10.096843 9.544824 7.748383

13 C 10.429041 9.234902 11.302442 10.537322 8.780403

14 H 2.085904 1.087973 2.561747 3.213603 2.182800

15 H 1.878666 3.193009 2.272556 0.967818 3.671233

16 H 3.465432 2.151390 4.499595 3.781818 1.091434

17 H 2.810036 2.154759 3.826389 2.917565 1.094227

18 H 2.826047 2.181648 4.022775 2.519409 1.087694

19 H 6.922998 5.766289 7.570165 7.376453 5.884370

20 H 7.065216 5.692499 7.808167 7.569855 5.522740

21 H 7.971138 6.722463 8.931757 8.065053 6.103335

22 H 7.851845 6.789196 8.730488 7.892831 6.436223

23 H 9.421272 8.248665 10.132498 9.736444 8.134906

24 H 9.533512 8.205613 10.317699 9.891263 7.888119

25 H 11.389946 10.175762 12.225068 11.551416 9.772562

26 H 10.529282 9.301808 11.473080 10.577556 8.678440

27 H 10.414593 9.327309 11.293104 10.420051 8.892451

6 7 8 9 10

6 S 0.000000

7 C 1.761125 0.000000

8 S 2.973843 1.795850 0.000000

9 S 3.057779 1.724347 3.096993 0.000000

10 C 4.360357 2.850178 1.836453 3.415702 0.000000

11 C 5.575707 4.211952 2.746795 4.890026 1.524524

12 C 6.843574 5.394704 4.160240 5.763874 2.545261

13 C 8.079302 6.716960 5.277916 7.204608 3.903714

14 H 2.435207 3.068122 4.463000 3.304433 5.836525

15 H 4.103718 5.637510 6.302814 6.745494 8.055881

16 H 3.045163 2.762804 3.115011 3.411542 4.653878

17 H 3.828505 4.212755 4.725896 4.816398 6.373088

18 H 3.073530 3.558107 3.613942 4.736002 5.421158

19 H 4.297160 2.962828 2.389995 3.517354 1.091145

20 H 4.715448 3.009466 2.420215 3.004507 1.087727

21 H 5.876155 4.495972 2.905856 5.141318 2.151084

22 H 5.552598 4.466914 2.887100 5.452501 2.152241

23 H 6.845027 5.488676 4.459676 5.851686 2.772920

24 H 7.119895 5.520310 4.483334 5.565968 2.776719

25 H 8.972012 7.565510 6.235428 7.908772 4.717634

26 H 8.339197 6.945386 5.413243 7.417135 4.230562

27 H 8.091643 6.907270 5.381050 7.622550 4.215759

11 12 13 14 15

11 C 0.000000

12 C 1.530386 0.000000

13 C 2.538194 1.528558 0.000000

14 H 7.110721 8.364505 9.633326 0.000000

15 H 8.949093 10.403254 11.386075 3.927078 0.000000

16 H 5.575865 6.950306 8.002831 2.512105 4.737186

17 H 7.259073 8.674551 9.673722 2.527028 3.749483

18 H 6.143631 7.640276 8.543367 3.095373 3.456601

19 H 2.174856 2.822839 4.239292 6.024331 8.181385

20 H 2.177485 2.824692 4.241430 5.793921 8.469063

21 H 1.095521 2.161464 2.764101 7.147849 8.965506

22 H 1.095165 2.154572 2.759778 7.337199 8.704077

23 H 2.155232 1.095119 2.157964 8.539287 10.550462

24 H 2.162763 1.094814 2.157967 8.387040 10.781906

25 H 3.493313 2.180016 1.092939 10.518708 12.398627

26 H 2.810669 2.182094 1.093590 9.709429 11.453497

27 H 2.793130 2.173562 1.093738 9.829109 11.222698

16 17 18 19 20

16 H 0.000000

17 H 1.766338 0.000000

18 H 1.767612 1.765979 0.000000

19 H 5.255218 6.908437 5.921156 0.000000

20 H 4.644322 6.403275 5.729050 1.767911 0.000000

21 H 5.297400 6.947820 5.902125 3.068964 2.519527

22 H 5.841683 7.418663 6.095779 2.510468 3.070497

23 H 7.403541 9.117232 8.044436 2.606416 3.148461

24 H 6.995198 8.752663 7.914322 3.148327 2.614275

25 H 8.966919 10.665401 9.580567 4.929638 4.935107

26 H 7.861860 9.494016 8.425538 4.797551 4.462809

27 H 8.217246 9.821069 8.536846 4.446632 4.785540

21 22 23 24 25

21 H 0.000000

22 H 1.752408 0.000000

23 H 3.061722 2.499249 0.000000

24 H 2.522134 3.061935 1.752646 0.000000

25 H 3.773670 3.762924 2.500377 2.502869 0.000000

26 H 2.589334 3.128473 3.078099 2.528333 1.764879

27 H 3.109915 2.565271 2.518976 3.072163 1.766966

26 27

26 H 0.000000

27 H 1.761722 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.18D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.084301 -0.477249 -0.123760

2 6 0 -2.824757 0.054621 0.485846

3 8 0 -4.885818 0.169374 -0.739238

4 8 0 -4.181607 -1.809167 -0.021670

5 6 0 -2.285562 -0.774807 1.639429

6 16 0 -1.604669 0.158441 -0.973107

7 6 0 -0.138513 0.755335 -0.201313

8 16 0 1.078826 -0.527905 0.109265

9 16 0 -0.001054 2.358064 0.419762

10 6 0 2.679094 0.326371 -0.176938

11 6 0 3.820534 -0.665833 0.014950

12 6 0 5.196317 -0.045313 -0.238540

13 6 0 6.328508 -1.052632 -0.038690

14 1 0 -3.029843 1.084344 0.770972

15 1 0 -5.003318 -2.082151 -0.454039

16 1 0 -1.369369 -0.323603 2.024440

17 1 0 -3.014934 -0.799961 2.454730

18 1 0 -2.068080 -1.800366 1.349588

19 1 0 2.651113 0.709024 -1.198403

20 1 0 2.757333 1.170168 0.504998

21 1 0 3.780218 -1.071287 1.031880

22 1 0 3.679934 -1.516756 -0.659993

23 1 0 5.231713 0.348285 -1.259870

24 1 0 5.345677 0.811319 0.426659

25 1 0 7.304460 -0.600438 -0.232478

26 1 0 6.341935 -1.445137 0.981946

27 1 0 6.214986 -1.905645 -0.713778

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2645617 0.1954460 0.1815636

Leave Link 202 at Sat Aug 17 17:51:23 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1103.1799811242 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0548518440 Hartrees.

Nuclear repulsion after empirical dispersion term = 1103.1251292802 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

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Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2329

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.58D-09

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 98

GePol: Fraction of low-weight points (<1% of avg) = 4.21%

GePol: Cavity surface area = 307.854 Ang\*\*2

GePol: Cavity volume = 319.503 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0056163343 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1103.1195129459 Hartrees.

Leave Link 301 at Sat Aug 17 17:51:23 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.86D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:51:23 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:51:24 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999859 -0.016740 -0.000271 -0.000948 Ang= -1.92 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.62968266463

Leave Link 401 at Sat Aug 17 17:51:24 2019, MaxMem= 1342177280 cpu: 8.0

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16272723.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.11D-15 for 2311.

Iteration 1 A\*A^-1 deviation from orthogonality is 6.20D-15 for 2302 849.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.77D-15 for 2311.

Iteration 1 A^-1\*A deviation from orthogonality is 1.80D-12 for 1585 1583.

E= -1658.63135730675

DIIS: error= 9.17D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.63135730675 IErMin= 1 ErrMin= 9.17D-03

ErrMax= 9.17D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.39D-02 BMatP= 9.39D-02

IDIUse=3 WtCom= 9.08D-01 WtEn= 9.17D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.429 Goal= None Shift= 0.000

Gap= 0.482 Goal= None Shift= 0.000

GapD= 0.429 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=6.11D-04 MaxDP=1.59D-02 OVMax= 5.20D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 6.11D-04 CP: 9.99D-01

E= -1658.67498925118 Delta-E= -0.043631944429 Rises=F Damp=F

DIIS: error= 9.41D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67498925118 IErMin= 2 ErrMin= 9.41D-04

ErrMax= 9.41D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.38D-03 BMatP= 9.39D-02

IDIUse=3 WtCom= 9.91D-01 WtEn= 9.41D-03

Coeff-Com: -0.637D-01 0.106D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.631D-01 0.106D+01

Gap= 0.129 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=1.26D-04 MaxDP=3.38D-03 DE=-4.36D-02 OVMax= 1.24D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.14D-04 CP: 9.99D-01 1.09D+00

E= -1658.67527098594 Delta-E= -0.000281734757 Rises=F Damp=F

DIIS: error= 6.70D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67527098594 IErMin= 3 ErrMin= 6.70D-04

ErrMax= 6.70D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.22D-03 BMatP= 1.38D-03

IDIUse=3 WtCom= 9.93D-01 WtEn= 6.70D-03

Coeff-Com: -0.412D-01 0.560D+00 0.481D+00

Coeff-En: 0.000D+00 0.145D+00 0.855D+00

Coeff: -0.410D-01 0.557D+00 0.484D+00

Gap= 0.126 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=8.12D-05 MaxDP=3.79D-03 DE=-2.82D-04 OVMax= 8.91D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 5.10D-05 CP: 9.99D-01 1.11D+00 4.60D-01

E= -1658.67551743958 Delta-E= -0.000246453645 Rises=F Damp=F

DIIS: error= 3.09D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67551743958 IErMin= 4 ErrMin= 3.09D-04

ErrMax= 3.09D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.26D-04 BMatP= 1.22D-03

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.09D-03

Coeff-Com: -0.142D-01 0.170D+00 0.308D+00 0.536D+00

Coeff-En: 0.000D+00 0.000D+00 0.182D+00 0.818D+00

Coeff: -0.141D-01 0.170D+00 0.308D+00 0.537D+00

Gap= 0.126 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=3.00D-05 MaxDP=1.56D-03 DE=-2.46D-04 OVMax= 3.13D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.58D-05 CP: 9.99D-01 1.11D+00 6.26D-01 6.65D-01

E= -1658.67557347693 Delta-E= -0.000056037350 Rises=F Damp=F

DIIS: error= 6.69D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67557347693 IErMin= 5 ErrMin= 6.69D-05

ErrMax= 6.69D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.57D-05 BMatP= 2.26D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.308D-02 0.305D-01 0.112D+00 0.287D+00 0.574D+00

Coeff: -0.308D-02 0.305D-01 0.112D+00 0.287D+00 0.574D+00

Gap= 0.126 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=6.76D-06 MaxDP=2.75D-04 DE=-5.60D-05 OVMax= 5.48D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 4.25D-06 CP: 9.99D-01 1.11D+00 6.32D-01 7.43D-01 7.98D-01

E= -1658.67557733823 Delta-E= -0.000003861297 Rises=F Damp=F

DIIS: error= 1.55D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67557733823 IErMin= 6 ErrMin= 1.55D-05

ErrMax= 1.55D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.50D-07 BMatP= 1.57D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.394D-03-0.828D-02 0.338D-02 0.422D-01 0.183D+00 0.780D+00

Coeff: 0.394D-03-0.828D-02 0.338D-02 0.422D-01 0.183D+00 0.780D+00

Gap= 0.126 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=2.50D-06 MaxDP=1.04D-04 DE=-3.86D-06 OVMax= 3.39D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.87D-06 CP: 9.99D-01 1.12D+00 6.40D-01 7.61D-01 8.60D-01

CP: 1.03D+00

E= -1658.67557752587 Delta-E= -0.000000187640 Rises=F Damp=F

DIIS: error= 5.98D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67557752587 IErMin= 7 ErrMin= 5.98D-06

ErrMax= 5.98D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.13D-07 BMatP= 5.50D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.413D-03-0.610D-02-0.817D-02-0.402D-02 0.316D-01 0.356D+00

Coeff-Com: 0.630D+00

Coeff: 0.413D-03-0.610D-02-0.817D-02-0.402D-02 0.316D-01 0.356D+00

Coeff: 0.630D+00

Gap= 0.126 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=9.91D-07 MaxDP=3.45D-05 DE=-1.88D-07 OVMax= 8.37D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 7.08D-07 CP: 9.99D-01 1.12D+00 6.41D-01 7.66D-01 8.82D-01

CP: 1.15D+00 9.73D-01

E= -1658.67557756426 Delta-E= -0.000000038395 Rises=F Damp=F

DIIS: error= 2.01D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67557756426 IErMin= 8 ErrMin= 2.01D-06

ErrMax= 2.01D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.40D-08 BMatP= 1.13D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.637D-04-0.332D-03-0.345D-02-0.794D-02-0.250D-01-0.267D-01

Coeff-Com: 0.216D+00 0.847D+00

Coeff: 0.637D-04-0.332D-03-0.345D-02-0.794D-02-0.250D-01-0.267D-01

Coeff: 0.216D+00 0.847D+00

Gap= 0.126 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=6.37D-07 MaxDP=2.55D-05 DE=-3.84D-08 OVMax= 8.85D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.37D-07 CP: 9.99D-01 1.12D+00 6.42D-01 7.69D-01 8.97D-01

CP: 1.23D+00 1.17D+00 1.04D+00

E= -1658.67557757207 Delta-E= -0.000000007808 Rises=F Damp=F

DIIS: error= 1.57D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67557757207 IErMin= 9 ErrMin= 1.57D-06

ErrMax= 1.57D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.46D-09 BMatP= 1.40D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.349D-04 0.820D-03-0.482D-03-0.307D-02-0.183D-01-0.710D-01

Coeff-Com: -0.605D-02 0.393D+00 0.705D+00

Coeff: -0.349D-04 0.820D-03-0.482D-03-0.307D-02-0.183D-01-0.710D-01

Coeff: -0.605D-02 0.393D+00 0.705D+00

Gap= 0.126 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=2.37D-07 MaxDP=1.05D-05 DE=-7.81D-09 OVMax= 3.07D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 8.38D-08 CP: 9.99D-01 1.12D+00 6.43D-01 7.70D-01 8.99D-01

CP: 1.25D+00 1.24D+00 1.21D+00 9.16D-01

E= -1658.67557757334 Delta-E= -0.000000001268 Rises=F Damp=F

DIIS: error= 8.29D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67557757334 IErMin=10 ErrMin= 8.29D-07

ErrMax= 8.29D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.36D-10 BMatP= 3.46D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.261D-04 0.460D-03 0.203D-03-0.416D-03-0.632D-02-0.344D-01

Coeff-Com: -0.372D-01 0.858D-01 0.388D+00 0.604D+00

Coeff: -0.261D-04 0.460D-03 0.203D-03-0.416D-03-0.632D-02-0.344D-01

Coeff: -0.372D-01 0.858D-01 0.388D+00 0.604D+00

Gap= 0.126 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=7.46D-08 MaxDP=2.86D-06 DE=-1.27D-09 OVMax= 6.68D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 3.90D-08 CP: 9.99D-01 1.12D+00 6.43D-01 7.70D-01 9.00D-01

CP: 1.26D+00 1.26D+00 1.26D+00 9.79D-01 9.26D-01

E= -1658.67557757352 Delta-E= -0.000000000180 Rises=F Damp=F

DIIS: error= 4.58D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67557757352 IErMin=11 ErrMin= 4.58D-07

ErrMax= 4.58D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.12D-10 BMatP= 7.36D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.880D-05 0.118D-03 0.182D-03 0.319D-03-0.503D-03-0.688D-02

Coeff-Com: -0.182D-01-0.137D-01 0.104D+00 0.327D+00 0.608D+00

Coeff: -0.880D-05 0.118D-03 0.182D-03 0.319D-03-0.503D-03-0.688D-02

Coeff: -0.182D-01-0.137D-01 0.104D+00 0.327D+00 0.608D+00

Gap= 0.126 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=2.45D-08 MaxDP=1.01D-06 DE=-1.80D-10 OVMax= 2.83D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.51D-08 CP: 9.99D-01 1.12D+00 6.43D-01 7.70D-01 9.00D-01

CP: 1.26D+00 1.26D+00 1.27D+00 1.03D+00 1.02D+00

CP: 8.59D-01

E= -1658.67557757353 Delta-E= -0.000000000011 Rises=F Damp=F

DIIS: error= 1.85D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.67557757353 IErMin=12 ErrMin= 1.85D-07

ErrMax= 1.85D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.93D-11 BMatP= 1.12D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.682D-06-0.113D-04 0.800D-04 0.309D-03 0.882D-03 0.218D-02

Coeff-Com: -0.448D-02-0.261D-01-0.640D-02 0.926D-01 0.382D+00 0.559D+00

Coeff: -0.682D-06-0.113D-04 0.800D-04 0.309D-03 0.882D-03 0.218D-02

Coeff: -0.448D-02-0.261D-01-0.640D-02 0.926D-01 0.382D+00 0.559D+00

Gap= 0.126 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=1.06D-08 MaxDP=4.04D-07 DE=-1.09D-11 OVMax= 8.55D-07

Cycle 13 Pass 1 IDiag 1:

RMSU= 6.60D-09 CP: 9.99D-01 1.12D+00 6.43D-01 7.70D-01 9.00D-01

CP: 1.26D+00 1.26D+00 1.27D+00 1.04D+00 1.07D+00

CP: 9.58D-01 7.87D-01

E= -1658.67557757354 Delta-E= -0.000000000011 Rises=F Damp=F

DIIS: error= 4.85D-08 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1658.67557757354 IErMin=13 ErrMin= 4.85D-08

ErrMax= 4.85D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.06D-12 BMatP= 2.93D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.124D-05-0.265D-04 0.483D-05 0.101D-03 0.522D-03 0.234D-02

Coeff-Com: 0.111D-02-0.106D-01-0.224D-01-0.150D-01 0.798D-01 0.284D+00

Coeff-Com: 0.680D+00

Coeff: 0.124D-05-0.265D-04 0.483D-05 0.101D-03 0.522D-03 0.234D-02

Coeff: 0.111D-02-0.106D-01-0.224D-01-0.150D-01 0.798D-01 0.284D+00

Coeff: 0.680D+00

Gap= 0.126 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=4.47D-09 MaxDP=1.48D-07 DE=-1.09D-11 OVMax= 3.61D-07

Error on total polarization charges = 0.04184

SCF Done: E(UB3LYP) = -1658.67557757 A.U. after 13 cycles

NFock= 13 Conv=0.45D-08 -V/T= 2.0020

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655332790293D+03 PE=-6.149101760064D+03 EE= 1.731973879252D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.52

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:51:53 2019, MaxMem= 1342177280 cpu: 329.7

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 341

Leave Link 701 at Sat Aug 17 17:51:54 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:51:54 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:51:57 2019, MaxMem= 1342177280 cpu: 38.3

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.36307427D+00-3.13143892D+00 4.68350678D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.013763111 -0.005263080 -0.002636487

2 6 -0.002175794 -0.002544955 0.000632579

3 8 -0.015053916 0.014756310 -0.004455250

4 8 -0.000250965 -0.011944298 0.004448082

5 6 0.001959904 0.005225637 0.002241489

6 16 0.003003201 0.000240495 0.003243658

7 6 0.000555219 -0.000176978 -0.000644956

8 16 -0.003227859 0.000649259 0.001166610

9 16 -0.000206785 -0.001544660 -0.000487670

10 6 -0.000968425 -0.001450935 -0.002899023

11 6 -0.000774793 0.000674160 0.000094391

12 6 0.000218737 -0.001437280 0.000489098

13 6 -0.000675966 0.000669966 -0.000749103

14 1 0.002603825 0.000588858 0.002087454

15 1 -0.002681842 -0.000350981 -0.002837772

16 1 -0.000077963 -0.000011526 0.000178368

17 1 -0.000072214 0.000110268 0.000490306

18 1 0.000262295 -0.000357731 -0.001921700

19 1 0.001756126 0.001394855 -0.000408234

20 1 0.000217129 0.000514082 0.001556816

21 1 0.000797379 -0.000000868 0.000788173

22 1 0.000445095 -0.000411204 -0.000665693

23 1 0.000165403 0.000382907 -0.000669420

24 1 -0.000543751 0.000518441 0.000890674

25 1 0.000757660 0.000056789 -0.000150522

26 1 -0.000248008 0.000134784 0.000990590

27 1 0.000453196 -0.000422314 -0.000772459

-------------------------------------------------------------------

Cartesian Forces: Max 0.015053916 RMS 0.003506259

Leave Link 716 at Sat Aug 17 17:51:57 2019, MaxMem= 1342177280 cpu: 0.3

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.020952105 RMS 0.002583516

Search for a local minimum.

Step number 47 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .25835D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43 45 44 47 46

ITU= 0 0 0 1 1 1 1 1 -1 -1 0 -1 -1 -1 0 -1 0 0 -1 -1

ITU= 0 0 -1 0 0 -1 1 -1 1 -1 1 1 -1 1 -1 1 1 -1 0 0

ITU= -1 0 0 -1 -1 0 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.98312.

Iteration 1 RMS(Cart)= 0.13031992 RMS(Int)= 0.00702380

Iteration 2 RMS(Cart)= 0.01612284 RMS(Int)= 0.00007694

Iteration 3 RMS(Cart)= 0.00014838 RMS(Int)= 0.00000266

Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00000266

ITry= 1 IFail=0 DXMaxC= 3.82D-01 DCOld= 1.00D+10 DXMaxT= 1.20D-01 DXLimC= 3.00D+00 Rises=T

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.82889 0.00688 0.00644 0.00000 0.00644 2.83532

R2 2.26717 0.02095 0.02217 0.00000 0.02217 2.28934

R3 2.53103 0.01232 0.02200 0.00000 0.02200 2.55303

R4 2.87178 -0.00189 -0.00657 0.00000 -0.00657 2.86521

R5 3.59939 -0.00021 0.01117 0.00000 0.01117 3.61056

R6 2.05597 0.00088 0.00215 0.00000 0.00215 2.05812

R7 1.82891 0.00373 0.00800 0.00000 0.00800 1.83691

R8 2.06251 0.00001 -0.00127 0.00000 -0.00127 2.06124

R9 2.06779 0.00039 0.00081 0.00000 0.00081 2.06860

R10 2.05544 0.00115 0.00460 0.00000 0.00460 2.06005

R11 3.32804 -0.00192 -0.01264 0.00000 -0.01264 3.31541

R12 3.39367 -0.00206 -0.00591 0.00000 -0.00591 3.38776

R13 3.25854 -0.00160 -0.00468 0.00000 -0.00468 3.25386

R14 3.47039 0.00181 0.00179 0.00000 0.00179 3.47218

R15 2.88093 0.00034 0.00043 0.00000 0.00043 2.88136

R16 2.06196 0.00102 0.00229 0.00000 0.00229 2.06426

R17 2.05551 0.00151 0.00454 0.00000 0.00454 2.06005

R18 2.89201 0.00007 0.00216 0.00000 0.00216 2.89417

R19 2.07023 0.00064 0.00196 0.00000 0.00196 2.07219

R20 2.06956 0.00071 0.00158 0.00000 0.00158 2.07115

R21 2.88856 -0.00011 -0.00231 0.00000 -0.00231 2.88624

R22 2.06948 0.00078 0.00246 0.00000 0.00246 2.07194

R23 2.06890 0.00092 0.00287 0.00000 0.00287 2.07177

R24 2.06535 0.00072 0.00228 0.00000 0.00228 2.06764

R25 2.06659 0.00079 0.00265 0.00000 0.00265 2.06923

R26 2.06687 0.00080 0.00217 0.00000 0.00217 2.06903

A1 2.18895 -0.00380 -0.01261 0.00000 -0.01260 2.17635

A2 1.96428 0.00299 0.01297 0.00000 0.01298 1.97726

A3 2.12532 0.00114 0.00365 0.00000 0.00366 2.12898

A4 1.99735 0.00420 0.02984 0.00000 0.02984 2.02719

A5 1.81977 0.00026 0.00909 0.00000 0.00909 1.82885

A6 1.85917 0.00014 0.01470 0.00000 0.01470 1.87386

A7 1.96483 -0.00245 -0.01763 0.00000 -0.01762 1.94721

A8 1.96548 -0.00273 -0.02408 0.00000 -0.02407 1.94141

A9 1.84408 0.00067 -0.01233 0.00000 -0.01233 1.83176

A10 1.88402 -0.00070 -0.01178 0.00000 -0.01178 1.87224

A11 1.91769 0.00042 -0.00477 0.00000 -0.00477 1.91293

A12 1.91946 0.00058 0.00684 0.00000 0.00684 1.92629

A13 1.96414 -0.00225 -0.01153 0.00000 -0.01153 1.95261

A14 1.88200 -0.00029 0.00139 0.00000 0.00139 1.88339

A15 1.89225 0.00065 0.00207 0.00000 0.00207 1.89432

A16 1.88615 0.00096 0.00653 0.00000 0.00653 1.89268

A17 1.78858 0.00185 0.01017 0.00000 0.01017 1.79876

A18 1.98006 -0.00005 -0.01006 0.00000 -0.01006 1.97000

A19 2.14032 0.00007 0.00244 0.00000 0.00244 2.14277

A20 2.15057 0.00000 0.00460 0.00000 0.00460 2.15517

A21 1.80425 -0.00199 -0.00862 0.00000 -0.00862 1.79563

A22 1.90716 0.00237 0.01924 0.00000 0.01924 1.92640

A23 1.86156 0.00096 0.01746 0.00000 0.01746 1.87902

A24 1.90269 -0.00133 -0.01056 0.00000 -0.01056 1.89213

A25 1.94472 -0.00123 -0.00551 0.00000 -0.00550 1.93921

A26 1.95208 -0.00103 -0.01372 0.00000 -0.01372 1.93836

A27 1.89304 0.00032 -0.00621 0.00000 -0.00621 1.88684

A28 1.96963 -0.00161 -0.01661 0.00000 -0.01661 1.95302

A29 1.90727 0.00086 0.00872 0.00000 0.00873 1.91599

A30 1.90921 0.00079 0.00783 0.00000 0.00783 1.91704

A31 1.91442 -0.00020 -0.00739 0.00000 -0.00739 1.90703

A32 1.90537 0.00030 0.00310 0.00000 0.00310 1.90847

A33 1.85438 -0.00006 0.00555 0.00000 0.00555 1.85992

A34 1.95736 0.00123 0.00868 0.00000 0.00868 1.96604

A35 1.90632 -0.00012 -0.00012 0.00000 -0.00011 1.90620

A36 1.91692 -0.00096 -0.00906 0.00000 -0.00906 1.90786

A37 1.91224 -0.00051 0.00064 0.00000 0.00064 1.91288

A38 1.91255 0.00005 0.00019 0.00000 0.00019 1.91274

A39 1.85566 0.00026 -0.00088 0.00000 -0.00088 1.85477

A40 1.94504 0.00036 0.00039 0.00000 0.00039 1.94544

A41 1.94727 -0.00095 -0.00507 0.00000 -0.00507 1.94220

A42 1.93519 0.00061 0.00762 0.00000 0.00762 1.94280

A43 1.87865 0.00012 -0.00171 0.00000 -0.00171 1.87694

A44 1.88170 -0.00050 -0.00452 0.00000 -0.00452 1.87718

A45 1.87277 0.00035 0.00312 0.00000 0.00312 1.87590

D1 2.73301 -0.00203 -0.01381 0.00000 -0.01381 2.71920

D2 -1.39622 -0.00239 -0.01087 0.00000 -0.01088 -1.40710

D3 0.54917 -0.00147 -0.01493 0.00000 -0.01493 0.53424

D4 -0.51087 0.00168 0.05200 0.00000 0.05200 -0.45887

D5 1.64309 0.00133 0.05493 0.00000 0.05493 1.69802

D6 -2.69471 0.00224 0.05087 0.00000 0.05088 -2.64383

D7 -3.11669 -0.00065 0.01631 0.00000 0.01631 -3.10037

D8 -0.07313 0.00258 0.07899 0.00000 0.07899 0.00586

D9 3.13902 -0.00004 0.00012 0.00000 0.00012 3.13914

D10 -1.07515 0.00022 0.00307 0.00000 0.00307 -1.07208

D11 1.02867 0.00034 0.00838 0.00000 0.00838 1.03705

D12 1.06521 -0.00160 -0.02017 0.00000 -0.02018 1.04503

D13 3.13422 -0.00134 -0.01723 0.00000 -0.01723 3.11699

D14 -1.04514 -0.00122 -0.01191 0.00000 -0.01192 -1.05706

D15 -1.01748 0.00122 0.02357 0.00000 0.02358 -0.99391

D16 1.05153 0.00148 0.02652 0.00000 0.02652 1.07806

D17 -3.12783 0.00160 0.03183 0.00000 0.03184 -3.09600

D18 -3.12274 -0.00082 0.03564 0.00000 0.03564 -3.08710

D19 -0.94782 0.00309 0.06808 0.00000 0.06809 -0.87974

D20 1.20416 -0.00134 0.02052 0.00000 0.02052 1.22468

D21 1.76950 0.00135 0.05405 0.00000 0.05405 1.82355

D22 -1.20948 0.00124 0.07241 0.00000 0.07241 -1.13707

D23 2.51457 0.00016 0.07905 0.00000 0.07905 2.59362

D24 -0.79073 0.00028 0.06030 0.00000 0.06030 -0.73043

D25 -3.11368 -0.00017 0.08604 0.00000 0.08604 -3.02764

D26 -1.00940 0.00024 0.10107 0.00000 0.10106 -0.90834

D27 1.03128 0.00045 0.09766 0.00000 0.09766 1.12894

D28 3.11711 0.00114 0.04189 0.00000 0.04189 -3.12419

D29 -1.03111 0.00042 0.02743 0.00000 0.02743 -1.00368

D30 0.99232 0.00128 0.04362 0.00000 0.04361 1.03594

D31 1.06444 -0.00078 0.01137 0.00000 0.01137 1.07581

D32 -3.08378 -0.00151 -0.00309 0.00000 -0.00309 -3.08687

D33 -1.06035 -0.00065 0.01310 0.00000 0.01310 -1.04725

D34 -1.05771 0.00041 0.03257 0.00000 0.03257 -1.02513

D35 1.07726 -0.00032 0.01811 0.00000 0.01811 1.09537

D36 3.10070 0.00054 0.03430 0.00000 0.03430 3.13499

D37 3.13932 -0.00005 0.01133 0.00000 0.01133 -3.13253

D38 -1.02058 0.00003 0.01785 0.00000 0.01785 -1.00273

D39 1.00820 -0.00027 0.01163 0.00000 0.01163 1.01984

D40 1.00837 0.00009 0.01662 0.00000 0.01662 1.02499

D41 3.13166 0.00017 0.02313 0.00000 0.02314 -3.12839

D42 -1.12274 -0.00013 0.01692 0.00000 0.01692 -1.10582

D43 -1.01692 0.00010 0.01237 0.00000 0.01237 -1.00455

D44 1.10637 0.00018 0.01888 0.00000 0.01888 1.12525

D45 3.13515 -0.00012 0.01267 0.00000 0.01267 -3.13537

D46 3.13142 0.00032 0.00541 0.00000 0.00541 3.13683

D47 -1.05120 0.00007 0.00003 0.00000 0.00003 -1.05117

D48 1.03521 0.00030 0.00571 0.00000 0.00571 1.04092

D49 1.01152 0.00001 -0.00073 0.00000 -0.00073 1.01079

D50 3.11209 -0.00024 -0.00610 0.00000 -0.00610 3.10598

D51 -1.08469 -0.00001 -0.00042 0.00000 -0.00042 -1.08512

D52 -1.01816 -0.00004 -0.00014 0.00000 -0.00014 -1.01830

D53 1.08240 -0.00029 -0.00551 0.00000 -0.00551 1.07689

D54 -3.11438 -0.00006 0.00017 0.00000 0.00017 -3.11421

Item Value Threshold Converged?

Maximum Force 0.020952 0.000450 NO

RMS Force 0.002584 0.000300 NO

Maximum Displacement 0.381994 0.001800 NO

RMS Displacement 0.142424 0.001200 NO

Predicted change in Energy=-7.104613D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:51:57 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.094175 -0.408082 -0.207333

2 6 0 -2.845165 0.074450 0.469646

3 8 0 -4.886154 0.305372 -0.783011

4 8 0 -4.244464 -1.749781 -0.157547

5 6 0 -2.301329 -0.807972 1.576194

6 16 0 -1.577278 0.290904 -0.943191

7 6 0 -0.116002 0.764328 -0.095492

8 16 0 1.083400 -0.563024 0.020411

9 16 0 0.020444 2.246209 0.770672

10 6 0 2.688020 0.331851 -0.000418

11 6 0 3.846469 -0.657051 -0.070697

12 6 0 5.203959 0.052017 -0.065182

13 6 0 6.376908 -0.922713 -0.147877

14 1 0 -3.039756 1.083750 0.829655

15 1 0 -5.053539 -1.968036 -0.650140

16 1 0 -1.396710 -0.360453 1.989899

17 1 0 -3.032709 -0.898345 2.385632

18 1 0 -2.059799 -1.808256 1.216367

19 1 0 2.685351 0.996882 -0.867004

20 1 0 2.751332 0.946163 0.897914

21 1 0 3.796059 -1.348590 0.778815

22 1 0 3.759587 -1.267940 -0.976506

23 1 0 5.248325 0.753127 -0.906977

24 1 0 5.292863 0.657885 0.844194

25 1 0 7.335961 -0.396053 -0.147427

26 1 0 6.379682 -1.614101 0.701228

27 1 0 6.330880 -1.524179 -1.061603

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.500388 0.000000

3 O 1.211467 2.405849 0.000000

4 O 1.351007 2.383113 2.242013 0.000000

5 C 2.560308 1.516204 3.672424 2.769230 0.000000

6 S 2.713823 1.910628 3.312782 3.448987 2.842372

7 C 4.148845 2.871174 4.841247 4.834128 3.168961

8 S 5.184897 4.005223 6.085653 5.461336 3.733209

9 S 4.993180 3.608167 5.500499 5.917683 3.920142

10 C 6.825576 5.559079 7.614543 7.239974 5.355232

11 C 7.945720 6.753149 8.814326 8.164851 6.366353

12 C 9.310595 8.066904 10.118786 9.619132 7.730656

13 C 10.483890 9.296359 11.347605 10.653528 8.848581

14 H 2.100645 1.089109 2.572110 3.233386 2.163610

15 H 1.884122 3.209765 2.283431 0.972052 3.725181

16 H 3.479427 2.144372 4.506503 3.827722 1.090761

17 H 2.844387 2.156967 3.863223 2.942967 1.094657

18 H 2.850630 2.172320 4.056256 2.581438 1.090129

19 H 6.954930 5.764037 7.603481 7.487978 5.838980

20 H 7.065162 5.680147 7.846484 7.571213 5.391330

21 H 8.007049 6.799007 8.975283 8.104798 6.173024

22 H 7.938045 6.893194 8.789857 8.060254 6.592613

23 H 9.440350 8.237735 10.145122 9.845772 8.099410

24 H 9.505707 8.167508 10.314284 9.887414 7.768933

25 H 11.430299 10.210655 12.258713 11.659285 9.798873

26 H 10.582138 9.380972 11.524166 10.659661 8.762155

27 H 10.519373 9.439287 11.368672 10.616314 9.054610

6 7 8 9 10

6 S 0.000000

7 C 1.754437 0.000000

8 S 2.955829 1.792725 0.000000

9 S 3.051763 1.721868 3.095893 0.000000

10 C 4.368440 2.838770 1.837401 3.372730 0.000000

11 C 5.574665 4.209763 2.766169 4.875991 1.524752

12 C 6.842013 5.367522 4.167086 5.690515 2.532281

13 C 8.085447 6.708705 5.308382 7.161734 3.899175

14 H 2.431138 3.083223 4.512999 3.274083 5.836249

15 H 4.156090 5.670337 6.331329 6.747139 8.102059

16 H 3.009965 2.693363 3.173463 3.207730 4.596267

17 H 3.822781 4.174643 4.759104 4.670981 6.319285

18 H 3.050080 3.481021 3.586169 4.578727 5.348122

19 H 4.321367 2.914943 2.405631 3.368164 1.092357

20 H 4.749304 3.039987 2.414467 3.027219 1.090132

21 H 5.875883 4.531342 2.924177 5.213244 2.158434

22 H 5.559967 4.463910 2.941552 5.420615 2.158781

23 H 6.841331 5.425370 4.465300 5.689863 2.748542

24 H 7.108323 5.490916 4.459688 5.506957 2.757694

25 H 8.975020 7.541945 6.257042 7.832065 4.706890

26 H 8.345440 6.963160 5.442323 7.439538 4.231714

27 H 8.114648 6.908902 5.443402 7.575926 4.223907

11 12 13 14 15

11 C 0.000000

12 C 1.531531 0.000000

13 C 2.545516 1.527333 0.000000

14 H 7.159687 8.356079 9.677553 0.000000

15 H 9.014687 10.470867 11.489129 3.944429 0.000000

16 H 5.641361 6.925484 8.081792 2.476184 4.788165

17 H 7.308548 8.645946 9.744750 2.519884 3.800514

18 H 6.153520 7.606915 8.592052 3.077915 3.531552

19 H 2.172048 2.806969 4.222509 5.971855 8.290247

20 H 2.169753 2.782523 4.210841 5.793124 8.473786

21 H 1.096558 2.157826 2.775051 7.255842 8.985601

22 H 1.096003 2.158474 2.766979 7.417799 8.846912

23 H 2.157120 1.096423 2.158326 8.474520 10.658288

24 H 2.158272 1.096332 2.158159 8.343508 10.778522

25 H 3.500081 2.180129 1.094146 10.526159 12.498943

26 H 2.815845 2.178453 1.094991 9.799016 11.518247

27 H 2.811780 2.178807 1.094886 9.908934 11.400496

16 17 18 19 20

16 H 0.000000

17 H 1.767039 0.000000

18 H 1.770359 1.772477 0.000000

19 H 5.164056 6.846002 5.892850 0.000000

20 H 4.483964 6.250652 5.552946 1.766879 0.000000

21 H 5.422914 7.029699 5.890146 3.073049 2.524190

22 H 6.017516 7.587876 6.242266 2.509063 3.071202

23 H 7.334061 9.063342 8.029816 2.574849 3.087048

24 H 6.862947 8.608893 7.764149 3.137234 2.558393

25 H 8.990494 10.685411 9.598675 4.907773 4.890103

26 H 7.981515 9.588672 8.457417 4.787971 4.445061

27 H 8.389373 9.997595 8.699042 4.436609 4.770269

21 22 23 24 25

21 H 0.000000

22 H 1.757551 0.000000

23 H 3.060749 2.511153 0.000000

24 H 2.504125 3.061811 1.754324 0.000000

25 H 3.781026 3.773329 2.501151 2.503667 0.000000

26 H 2.598388 3.130418 3.077347 2.522605 1.765879

27 H 3.137401 2.585430 2.526254 3.077490 1.765949

26 27

26 H 0.000000

27 H 1.765798 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.15D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.103523 -0.464256 -0.131040

2 6 0 -2.848992 0.120742 0.447832

3 8 0 -4.899607 0.146283 -0.810117

4 8 0 -4.254134 -1.779238 0.139805

5 6 0 -2.296975 -0.568740 1.680215

6 16 0 -1.592095 0.099677 -0.991010

7 6 0 -0.123972 0.703371 -0.243870

8 16 0 1.075593 -0.589039 0.079521

9 16 0 0.020045 2.307238 0.365802

10 6 0 2.680478 0.287323 -0.100409

11 6 0 3.837813 -0.701777 -0.015993

12 6 0 5.195683 -0.003914 -0.137501

13 6 0 6.367427 -0.981103 -0.067772

14 1 0 -3.040219 1.175846 0.638478

15 1 0 -5.067159 -2.074040 -0.304005

16 1 0 -1.388905 -0.060939 2.007791

17 1 0 -3.022041 -0.523484 2.499060

18 1 0 -2.058805 -1.615007 1.487908

19 1 0 2.671375 0.800841 -1.064495

20 1 0 2.751152 1.040848 0.684188

21 1 0 3.793691 -1.244153 0.936016

22 1 0 3.743513 -1.453112 -0.808347

23 1 0 5.233827 0.549182 -1.083425

24 1 0 5.292031 0.743052 0.659182

25 1 0 7.326736 -0.463275 -0.161243

26 1 0 6.376484 -1.523492 0.883404

27 1 0 6.313923 -1.724518 -0.869798

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3046154 0.1933921 0.1809013

Leave Link 202 at Sat Aug 17 17:51:57 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.3455620100 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0550007793 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.2905612307 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2322

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.11D-09

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 95

GePol: Fraction of low-weight points (<1% of avg) = 4.09%

GePol: Cavity surface area = 309.143 Ang\*\*2

GePol: Cavity volume = 320.360 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057819032 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.2847793274 Hartrees.

Leave Link 301 at Sat Aug 17 17:51:57 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:51:57 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:51:57 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Lowest energy guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000312 -0.000004 -0.000016 Ang= -0.04 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999865 0.016426 0.000267 0.000932 Ang= 1.89 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 1.69D-02

Max alpha theta= 3.607 degrees.

Max beta theta= 3.607 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 17:51:58 2019, MaxMem= 1342177280 cpu: 4.4

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16175052.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.33D-15 for 2315.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.02D-15 for 707 445.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.44D-15 for 2315.

Iteration 1 A^-1\*A deviation from orthogonality is 1.05D-08 for 915 742.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.55D-15 for 377.

Iteration 2 A\*A^-1 deviation from orthogonality is 1.86D-15 for 700 434.

Iteration 2 A^-1\*A deviation from unit magnitude is 9.99D-16 for 56.

Iteration 2 A^-1\*A deviation from orthogonality is 3.36D-16 for 962 9.

E= -1658.67701540117

DIIS: error= 2.12D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67701540117 IErMin= 1 ErrMin= 2.12D-05

ErrMax= 2.12D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.46D-07 BMatP= 2.46D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 88.942 Goal= None Shift= 0.000

Gap= 88.954 Goal= None Shift= 0.000

RMSDP=8.68D-07 MaxDP=2.73D-05 OVMax= 6.25D-05

Cycle 2 Pass 1 IDiag 1:

RMSU= 8.67D-07 CP: 1.00D+00

E= -1658.67701545778 Delta-E= -0.000000056604 Rises=F Damp=F

DIIS: error= 1.01D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67701545778 IErMin= 2 ErrMin= 1.01D-05

ErrMax= 1.01D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.33D-08 BMatP= 2.46D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.298D+00 0.702D+00

Coeff: 0.298D+00 0.702D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.42D-07 MaxDP=3.27D-05 DE=-5.66D-08 OVMax= 4.12D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 4.75D-07 CP: 1.00D+00 6.99D-01

E= -1658.67701546115 Delta-E= -0.000000003376 Rises=F Damp=F

DIIS: error= 9.33D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67701546115 IErMin= 3 ErrMin= 9.33D-06

ErrMax= 9.33D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.68D-08 BMatP= 8.33D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.232D-01 0.477D+00 0.547D+00

Coeff: -0.232D-01 0.477D+00 0.547D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.61D-07 MaxDP=1.70D-05 DE=-3.38D-09 OVMax= 2.47D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 8.51D-08 CP: 1.00D+00 8.62D-01 5.74D-01

E= -1658.67701547248 Delta-E= -0.000000011326 Rises=F Damp=F

DIIS: error= 1.57D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67701547248 IErMin= 4 ErrMin= 1.57D-06

ErrMax= 1.57D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.85D-09 BMatP= 6.68D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.198D-01 0.268D+00 0.320D+00 0.432D+00

Coeff: -0.198D-01 0.268D+00 0.320D+00 0.432D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.51D-08 MaxDP=3.16D-06 DE=-1.13D-08 OVMax= 5.59D-06

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.63D-08 CP: 1.00D+00 8.64D-01 5.94D-01 5.28D-01

E= -1658.67701547281 Delta-E= -0.000000000329 Rises=F Damp=F

DIIS: error= 5.27D-07 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67701547281 IErMin= 5 ErrMin= 5.27D-07

ErrMax= 5.27D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.63D-10 BMatP= 1.85D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.814D-02 0.967D-01 0.117D+00 0.260D+00 0.535D+00

Coeff: -0.814D-02 0.967D-01 0.117D+00 0.260D+00 0.535D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.81D-08 MaxDP=8.54D-07 DE=-3.29D-10 OVMax= 1.63D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.38D-08 CP: 1.00D+00 8.66D-01 5.91D-01 5.90D-01 7.26D-01

E= -1658.67701547284 Delta-E= -0.000000000035 Rises=F Damp=F

DIIS: error= 8.83D-08 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67701547284 IErMin= 6 ErrMin= 8.83D-08

ErrMax= 8.83D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.13D-11 BMatP= 1.63D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.187D-02 0.184D-01 0.222D-01 0.862D-01 0.273D+00 0.602D+00

Coeff: -0.187D-02 0.184D-01 0.222D-01 0.862D-01 0.273D+00 0.602D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.86D-09 MaxDP=2.57D-07 DE=-3.50D-11 OVMax= 6.28D-07

Error on total polarization charges = 0.04162

SCF Done: E(UB3LYP) = -1658.67701547 A.U. after 6 cycles

NFock= 6 Conv=0.59D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655236418719D+03 PE=-6.147336364793D+03 EE= 1.731138151274D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.63

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:52:13 2019, MaxMem= 1342177280 cpu: 174.4

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 337

Leave Link 701 at Sat Aug 17 17:52:14 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:52:14 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:52:17 2019, MaxMem= 1342177280 cpu: 38.4

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.40741562D+00-2.94311817D+00 6.40614913D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000009534 0.000010526 -0.000060430

2 6 0.000029121 -0.000042644 0.000066205

3 8 -0.000059312 0.000085821 0.000040323

4 8 -0.000007121 -0.000068259 -0.000010193

5 6 0.000008538 0.000015531 0.000009707

6 16 0.000100960 0.000056394 0.000039565

7 6 -0.000059748 -0.000000903 0.000038032

8 16 -0.000033015 0.000002421 -0.000004790

9 16 -0.000001756 -0.000037867 0.000042240

10 6 0.000014812 -0.000007041 -0.000018555

11 6 -0.000003089 0.000018052 -0.000005122

12 6 -0.000005076 -0.000008832 -0.000002677

13 6 -0.000003810 0.000017151 -0.000015378

14 1 -0.000002666 -0.000009822 0.000051538

15 1 -0.000017513 0.000025352 -0.000055331

16 1 0.000021858 -0.000037592 0.000002615

17 1 0.000001591 -0.000049282 -0.000004810

18 1 0.000007781 -0.000017422 -0.000063271

19 1 0.000025338 0.000033982 0.000025185

20 1 -0.000018928 -0.000018955 0.000042919

21 1 0.000015211 -0.000012810 -0.000025386

22 1 0.000000308 0.000015045 -0.000029028

23 1 0.000003816 0.000020720 0.000015361

24 1 -0.000007264 -0.000008145 0.000025765

25 1 0.000006374 0.000006100 -0.000016317

26 1 -0.000008490 -0.000014538 -0.000036963

27 1 0.000001614 0.000027017 -0.000051203

-------------------------------------------------------------------

Cartesian Forces: Max 0.000100960 RMS 0.000032196

Leave Link 716 at Sat Aug 17 17:52:17 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000104377 RMS 0.000025449

Search for a local minimum.

Step number 48 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .25449D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43 45 44 47 46

48

ITU= 0 0 0 0 1 1 1 1 1 -1 -1 0 -1 -1 -1 0 -1 0 0 -1

ITU= -1 0 0 -1 0 0 -1 1 -1 1 -1 1 1 -1 1 -1 1 1 -1 0

ITU= 0 -1 0 0 -1 -1 0 0

Use linear search instead of GDIIS.

Eigenvalues --- -0.00429 0.00000 0.00004 0.00050 0.00235

Eigenvalues --- 0.00322 0.00389 0.00656 0.00906 0.01906

Eigenvalues --- 0.02241 0.03249 0.03388 0.03850 0.04154

Eigenvalues --- 0.04502 0.04796 0.04862 0.05035 0.05428

Eigenvalues --- 0.05455 0.05564 0.05598 0.05888 0.06970

Eigenvalues --- 0.08164 0.08329 0.10876 0.11332 0.11554

Eigenvalues --- 0.12498 0.13975 0.14953 0.15166 0.15835

Eigenvalues --- 0.15978 0.16011 0.16220 0.16644 0.17459

Eigenvalues --- 0.18315 0.19306 0.20300 0.21512 0.22212

Eigenvalues --- 0.22680 0.23117 0.24459 0.24998 0.25329

Eigenvalues --- 0.27030 0.28851 0.29108 0.29481 0.29654

Eigenvalues --- 0.31066 0.31560 0.32360 0.33322 0.33875

Eigenvalues --- 0.33885 0.33942 0.33969 0.34031 0.34062

Eigenvalues --- 0.34101 0.34219 0.34273 0.34676 0.34794

Eigenvalues --- 0.35167 0.36265 0.47591 0.52463 0.82923

Eigenvalue 1 is -4.29D-03 should be greater than 0.000000 Eigenvector:

D25 D27 D26 D22 D2

1 -0.45091 -0.39640 -0.38492 -0.30861 -0.25371

D23 D3 D1 D8 D5

1 -0.24894 -0.23728 -0.21980 0.16716 -0.12538

RFO step: Lambda=-4.28992215D-03 EMin=-4.28660516D-03

I= 1 Eig= -4.29D-03 Dot1= 3.57D-05

I= 1 Stepn= 2.99D-01 RXN= 2.99D-01 EDone=F

Mixed 1 eigenvectors in step. Raw Step.Grad= 3.57D-05.

RFO eigenvector is Hessian eigenvector with negative curvature.

Taking step of 2.99D-01 in eigenvector direction(s). Step.Grad= -1.46D-05.

Quartic linear search produced a step of -0.01542.

Iteration 1 RMS(Cart)= 0.11684604 RMS(Int)= 0.00508825

Iteration 2 RMS(Cart)= 0.00912600 RMS(Int)= 0.00012019

Iteration 3 RMS(Cart)= 0.00004610 RMS(Int)= 0.00011923

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00011923

ITry= 1 IFail=0 DXMaxC= 3.48D-01 DCOld= 1.00D+10 DXMaxT= 1.20D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83532 0.00010 0.00000 0.01378 0.01378 2.84910

R2 2.28934 0.00006 0.00001 -0.00387 -0.00386 2.28548

R3 2.55303 0.00008 0.00001 0.00516 0.00517 2.55820

R4 2.86521 -0.00003 0.00000 -0.00421 -0.00421 2.86100

R5 3.61056 0.00002 0.00000 -0.00400 -0.00400 3.60657

R6 2.05812 0.00001 0.00000 -0.00122 -0.00122 2.05690

R7 1.83691 0.00002 0.00000 0.00093 0.00093 1.83784

R8 2.06124 0.00002 0.00000 0.00116 0.00116 2.06240

R9 2.06860 0.00000 0.00000 0.00017 0.00017 2.06877

R10 2.06005 0.00001 0.00000 0.00163 0.00163 2.06168

R11 3.31541 -0.00008 0.00000 -0.01242 -0.01242 3.30298

R12 3.38776 0.00000 0.00000 -0.00347 -0.00347 3.38429

R13 3.25386 -0.00003 0.00000 -0.00407 -0.00407 3.24979

R14 3.47218 0.00002 0.00000 0.00591 0.00591 3.47809

R15 2.88136 0.00000 0.00000 -0.00153 -0.00153 2.87983

R16 2.06426 0.00001 0.00000 -0.00042 -0.00042 2.06384

R17 2.06005 0.00001 0.00000 0.00162 0.00163 2.06168

R18 2.89417 -0.00001 0.00000 -0.00258 -0.00258 2.89160

R19 2.07219 0.00000 0.00000 -0.00089 -0.00089 2.07131

R20 2.07115 0.00001 0.00000 -0.00095 -0.00094 2.07020

R21 2.88624 -0.00001 0.00000 -0.00059 -0.00059 2.88565

R22 2.07194 0.00000 0.00000 -0.00198 -0.00198 2.06995

R23 2.07177 0.00001 0.00000 0.00092 0.00092 2.07269

R24 2.06764 0.00001 0.00000 -0.00029 -0.00029 2.06735

R25 2.06923 0.00000 0.00000 -0.00153 -0.00153 2.06771

R26 2.06903 0.00001 0.00000 0.00091 0.00092 2.06995

A1 2.17635 -0.00004 0.00000 0.00237 0.00215 2.17850

A2 1.97726 0.00005 0.00000 0.00577 0.00556 1.98282

A3 2.12898 0.00000 0.00000 -0.00689 -0.00711 2.12187

A4 2.02719 0.00007 0.00001 0.01248 0.01254 2.03973

A5 1.82885 0.00003 0.00000 0.01255 0.01264 1.84150

A6 1.87386 -0.00003 0.00000 -0.00004 -0.00005 1.87382

A7 1.94721 -0.00008 0.00000 -0.02159 -0.02167 1.92554

A8 1.94141 -0.00002 -0.00001 -0.00287 -0.00298 1.93843

A9 1.83176 0.00003 0.00000 -0.00050 -0.00063 1.83113

A10 1.87224 -0.00001 0.00000 -0.00298 -0.00299 1.86926

A11 1.91293 0.00000 0.00000 0.00707 0.00702 1.91995

A12 1.92629 0.00001 0.00000 0.00710 0.00708 1.93337

A13 1.95261 -0.00004 0.00000 -0.01536 -0.01535 1.93726

A14 1.88339 0.00000 0.00000 0.00359 0.00351 1.88690

A15 1.89432 0.00001 0.00000 -0.00570 -0.00571 1.88861

A16 1.89268 0.00002 0.00000 0.00369 0.00372 1.89640

A17 1.79876 -0.00006 0.00000 -0.00229 -0.00228 1.79647

A18 1.97000 0.00002 0.00000 0.00821 0.00752 1.97752

A19 2.14277 -0.00002 0.00000 0.00434 0.00365 2.14642

A20 2.15517 -0.00001 0.00000 -0.00133 -0.00202 2.15315

A21 1.79563 -0.00002 0.00000 -0.00872 -0.00872 1.78690

A22 1.92640 0.00005 0.00001 0.01038 0.01031 1.93671

A23 1.87902 0.00000 0.00000 0.01119 0.01106 1.89008

A24 1.89213 -0.00003 0.00000 -0.00626 -0.00622 1.88591

A25 1.93921 -0.00001 0.00000 0.00529 0.00515 1.94436

A26 1.93836 -0.00001 0.00000 -0.01518 -0.01517 1.92318

A27 1.88684 0.00001 0.00000 -0.00520 -0.00519 1.88165

A28 1.95302 -0.00003 0.00000 -0.00357 -0.00358 1.94944

A29 1.91599 0.00001 0.00000 -0.00005 -0.00008 1.91591

A30 1.91704 0.00002 0.00000 0.00703 0.00703 1.92406

A31 1.90703 0.00000 0.00000 -0.00529 -0.00530 1.90173

A32 1.90847 0.00001 0.00000 -0.00173 -0.00172 1.90675

A33 1.85992 -0.00001 0.00000 0.00392 0.00390 1.86383

A34 1.96604 0.00001 0.00000 0.00071 0.00070 1.96675

A35 1.90620 0.00000 0.00000 -0.00272 -0.00272 1.90348

A36 1.90786 -0.00001 0.00000 -0.00125 -0.00126 1.90660

A37 1.91288 -0.00001 0.00000 -0.00337 -0.00337 1.90950

A38 1.91274 0.00000 0.00000 0.00645 0.00646 1.91920

A39 1.85477 0.00000 0.00000 0.00011 0.00012 1.85489

A40 1.94544 0.00001 0.00000 0.00237 0.00237 1.94781

A41 1.94220 -0.00001 0.00000 -0.00476 -0.00476 1.93743

A42 1.94280 0.00000 0.00000 0.00014 0.00014 1.94294

A43 1.87694 0.00000 0.00000 0.00065 0.00065 1.87759

A44 1.87718 -0.00001 0.00000 -0.00330 -0.00330 1.87388

A45 1.87590 0.00001 0.00000 0.00507 0.00507 1.88097

D1 2.71920 -0.00001 0.00000 -0.06576 -0.06583 2.65338

D2 -1.40710 -0.00005 0.00000 -0.07591 -0.07589 -1.48299

D3 0.53424 -0.00002 0.00000 -0.07099 -0.07103 0.46321

D4 -0.45887 0.00001 0.00001 -0.02737 -0.02736 -0.48623

D5 1.69802 -0.00003 0.00001 -0.03751 -0.03743 1.66059

D6 -2.64383 0.00000 0.00001 -0.03260 -0.03257 -2.67640

D7 -3.10037 0.00000 0.00000 0.01259 0.01267 -3.08770

D8 0.00586 0.00002 0.00002 0.05001 0.04995 0.05581

D9 3.13914 0.00000 0.00000 -0.00071 -0.00076 3.13839

D10 -1.07208 0.00001 0.00000 0.01240 0.01240 -1.05968

D11 1.03705 0.00002 0.00000 0.01166 0.01163 1.04868

D12 1.04503 -0.00002 -0.00001 -0.00956 -0.00952 1.03551

D13 3.11699 -0.00002 0.00000 0.00355 0.00364 3.12063

D14 -1.05706 -0.00001 0.00000 0.00281 0.00287 -1.05420

D15 -0.99391 0.00000 0.00001 0.00662 0.00657 -0.98734

D16 1.07806 0.00001 0.00001 0.01972 0.01973 1.09778

D17 -3.09600 0.00001 0.00001 0.01899 0.01895 -3.07704

D18 -3.08710 -0.00003 0.00001 -0.01787 -0.01782 -3.10493

D19 -0.87974 0.00003 0.00002 -0.00716 -0.00720 -0.88694

D20 1.22468 -0.00002 0.00001 -0.02267 -0.02264 1.20204

D21 1.82355 -0.00004 0.00001 -0.02654 -0.02643 1.79712

D22 -1.13707 -0.00003 0.00002 -0.09233 -0.09241 -1.22949

D23 2.59362 0.00000 0.00002 -0.07448 -0.07443 2.51919

D24 -0.73043 -0.00001 0.00002 -0.00746 -0.00747 -0.73790

D25 -3.02764 -0.00004 0.00002 -0.13491 -0.13495 3.12059

D26 -0.90834 -0.00002 0.00003 -0.11516 -0.11506 -1.02340

D27 1.12894 -0.00003 0.00003 -0.11860 -0.11859 1.01036

D28 -3.12419 0.00001 0.00001 0.00272 0.00277 -3.12142

D29 -1.00368 0.00000 0.00001 -0.00640 -0.00636 -1.01004

D30 1.03594 0.00001 0.00001 0.00244 0.00249 1.03843

D31 1.07581 -0.00001 0.00000 -0.02143 -0.02145 1.05435

D32 -3.08687 -0.00002 0.00000 -0.03055 -0.03058 -3.11745

D33 -1.04725 -0.00001 0.00000 -0.02172 -0.02173 -1.06898

D34 -1.02513 0.00000 0.00001 -0.00819 -0.00820 -1.03333

D35 1.09537 -0.00001 0.00000 -0.01731 -0.01733 1.07805

D36 3.13499 0.00000 0.00001 -0.00847 -0.00847 3.12652

D37 -3.13253 -0.00001 0.00000 0.00880 0.00880 -3.12373

D38 -1.00273 -0.00001 0.00000 0.00304 0.00305 -0.99967

D39 1.01984 -0.00001 0.00000 0.00097 0.00098 1.02082

D40 1.02499 0.00000 0.00000 0.01486 0.01486 1.03985

D41 -3.12839 0.00000 0.00001 0.00911 0.00911 -3.11928

D42 -1.10582 0.00000 0.00000 0.00703 0.00703 -1.09879

D43 -1.00455 0.00000 0.00000 0.01412 0.01413 -0.99043

D44 1.12525 0.00000 0.00001 0.00837 0.00837 1.13363

D45 -3.13537 0.00000 0.00000 0.00629 0.00630 -3.12907

D46 3.13683 0.00000 0.00000 -0.00756 -0.00756 3.12927

D47 -1.05117 0.00000 0.00000 -0.00837 -0.00837 -1.05954

D48 1.04092 0.00000 0.00000 -0.00506 -0.00506 1.03585

D49 1.01079 0.00000 0.00000 -0.00216 -0.00217 1.00863

D50 3.10598 0.00000 0.00000 -0.00298 -0.00298 3.10300

D51 -1.08512 0.00000 0.00000 0.00033 0.00033 -1.08479

D52 -1.01830 0.00000 0.00000 -0.00407 -0.00406 -1.02236

D53 1.07689 0.00000 0.00000 -0.00488 -0.00487 1.07202

D54 -3.11421 0.00000 0.00000 -0.00157 -0.00157 -3.11578

Item Value Threshold Converged?

Maximum Force 0.000104 0.000450 YES

RMS Force 0.000025 0.000300 YES

Maximum Displacement 0.348365 0.001800 NO

RMS Displacement 0.120664 0.001200 NO

Predicted change in Energy=-2.253977D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:52:18 2019, MaxMem= 1342177280 cpu: 0.6

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.118022 -0.349731 -0.164587

2 6 0 -2.835815 0.061989 0.513296

3 8 0 -4.946667 0.416837 -0.598664

4 8 0 -4.278685 -1.691075 -0.251754

5 6 0 -2.259505 -0.900763 1.529713

6 16 0 -1.586358 0.362791 -0.897659

7 6 0 -0.119398 0.772612 -0.040276

8 16 0 1.064228 -0.570000 0.020630

9 16 0 0.085388 2.253338 0.809979

10 6 0 2.672761 0.316062 -0.102075

11 6 0 3.840064 -0.661556 -0.038285

12 6 0 5.187213 0.060529 -0.110352

13 6 0 6.373290 -0.900531 -0.073321

14 1 0 -3.002067 1.043159 0.954226

15 1 0 -5.102581 -1.849035 -0.743778

16 1 0 -1.335730 -0.495336 1.946087

17 1 0 -2.962098 -1.062136 2.353599

18 1 0 -2.032602 -1.864181 1.070791

19 1 0 2.680249 0.885485 -1.033990

20 1 0 2.731195 1.026686 0.723674

21 1 0 3.792855 -1.235089 0.894583

22 1 0 3.773768 -1.385023 -0.858241

23 1 0 5.227007 0.652450 -1.031160

24 1 0 5.258744 0.775688 0.718167

25 1 0 7.326150 -0.366995 -0.138292

26 1 0 6.380904 -1.478567 0.855685

27 1 0 6.337871 -1.609244 -0.907771

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.507679 0.000000

3 O 1.209423 2.412068 0.000000

4 O 1.353741 2.395916 2.238268 0.000000

5 C 2.574563 1.513978 3.672452 2.806298 0.000000

6 S 2.730275 1.908512 3.374018 3.447345 2.818125

7 C 4.155009 2.861878 4.872463 4.838816 3.137691

8 S 5.190234 3.981515 6.122763 5.466052 3.665233

9 S 5.039286 3.663803 5.538826 5.977525 3.995609

10 C 6.823629 5.548661 7.636258 7.236961 5.335788

11 C 7.965194 6.737589 8.870377 8.186547 6.302426

12 C 9.314432 8.047230 10.151893 9.627634 7.685538

13 C 10.506157 9.277833 11.408457 10.682761 8.780368

14 H 2.106477 1.088464 2.566168 3.249643 2.159032

15 H 1.884869 3.220323 2.275861 0.972545 3.761790

16 H 3.495324 2.147965 4.510730 3.862807 1.091374

17 H 2.860934 2.160166 3.852497 2.986106 1.094745

18 H 2.858092 2.160112 4.059790 2.612274 1.090994

19 H 6.964058 5.787849 7.653692 7.461724 5.845034

20 H 7.042393 5.653892 7.814733 7.581300 5.410346

21 H 8.030422 6.765135 9.018753 8.165279 6.094770

22 H 7.989576 6.903734 8.908426 8.081057 6.506705

23 H 9.438479 8.230619 10.185589 9.821292 8.063399

24 H 9.485229 8.128544 10.296273 9.898900 7.745525

25 H 11.444215 10.191866 12.306437 11.680679 9.744328

26 H 10.608613 9.350853 11.576768 10.719068 8.685899

27 H 10.557670 9.432336 11.469148 10.637120 8.964270

6 7 8 9 10

6 S 0.000000

7 C 1.747864 0.000000

8 S 2.956173 1.790890 0.000000

9 S 3.047118 1.719715 3.090701 0.000000

10 C 4.333039 2.829913 1.840527 3.358479 0.000000

11 C 5.588726 4.211197 2.777970 4.828431 1.523943

12 C 6.825868 5.354633 4.172976 5.628857 2.527417

13 C 8.101328 6.704887 5.320172 7.089769 3.895491

14 H 2.428294 3.061373 4.473101 3.319294 5.817913

15 H 4.156883 5.674509 6.344271 6.794015 8.096626

16 H 2.980954 2.651941 3.077784 3.296290 4.573984

17 H 3.807067 4.144620 4.679341 4.760494 6.299317

18 H 3.005551 3.442019 3.516831 4.637658 5.316909

19 H 4.300667 2.972917 2.417061 3.464758 1.092137

20 H 4.659479 2.962103 2.412977 2.917605 1.090992

21 H 5.890780 4.495615 2.941351 5.091326 2.157315

22 H 5.638028 4.525616 2.962817 5.442865 2.162798

23 H 6.820826 5.438782 4.464234 5.691123 2.738710

24 H 7.045339 5.431359 4.459978 5.381031 2.751612

25 H 8.974521 7.532895 6.267228 7.758480 4.703394

26 H 8.363138 6.937182 5.458009 7.318657 4.229460

27 H 8.165931 6.937010 5.454656 7.547433 4.217699

11 12 13 14 15

11 C 0.000000

12 C 1.530167 0.000000

13 C 2.544715 1.527020 0.000000

14 H 7.120806 8.316441 9.629699 0.000000

15 H 9.048686 10.484632 11.534504 3.957293 0.000000

16 H 5.545647 6.861976 7.979423 2.475365 4.822555

17 H 7.221563 8.587357 9.647048 2.528263 3.846378

18 H 6.096274 7.564743 8.537953 3.066933 3.566183

19 H 2.174841 2.796162 4.213228 6.022174 8.254348

20 H 2.158780 2.767866 4.196931 5.737919 8.472970

21 H 1.096089 2.152383 2.776223 7.166934 9.065867

22 H 1.095503 2.155641 2.758324 7.422468 8.889205

23 H 2.153143 1.095373 2.154802 8.474200 10.632046

24 H 2.156512 1.096819 2.162956 8.268510 10.788119

25 H 3.499938 2.181424 1.093994 10.481135 12.531417

26 H 2.814705 2.174154 1.094183 9.716427 11.600257

27 H 2.809477 2.178999 1.095370 9.886188 11.444140

16 17 18 19 20

16 H 0.000000

17 H 1.769859 0.000000

18 H 1.767911 1.775622 0.000000

19 H 5.188026 6.863313 5.848225 0.000000

20 H 4.511178 6.279603 5.583132 1.764062 0.000000

21 H 5.287276 6.912889 5.861976 3.074755 2.504388

22 H 5.895995 7.469408 6.137156 2.526238 3.066880

23 H 7.297324 9.025400 7.965775 2.557399 3.073854

24 H 6.827180 8.581053 7.762537 3.119414 2.539988

25 H 8.910066 10.608524 9.554564 4.894423 4.878417

26 H 7.855073 9.471476 8.425085 4.780634 4.428781

27 H 8.262533 9.870425 8.604913 4.429199 4.755823

21 22 23 24 25

21 H 0.000000

22 H 1.759328 0.000000

23 H 3.054191 2.508606 0.000000

24 H 2.494629 3.059230 1.753950 0.000000

25 H 3.782141 3.764855 2.498576 2.512651 0.000000

26 H 2.599768 3.121451 3.071302 2.521868 1.765523

27 H 3.140951 2.574365 2.522797 3.081573 1.764079

26 27

26 H 0.000000

27 H 1.768815 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.65D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.123834 -0.432822 -0.122778

2 6 0 -2.838793 0.080541 0.475738

3 8 0 -4.957215 0.256422 -0.664185

4 8 0 -4.281209 -1.771942 -0.001917

5 6 0 -2.253724 -0.713603 1.624284

6 16 0 -1.598603 0.163445 -0.972528

7 6 0 -0.127741 0.702847 -0.197519

8 16 0 1.060028 -0.612245 0.061370

9 16 0 0.077897 2.296970 0.413960

10 6 0 2.665285 0.247497 -0.206091

11 6 0 3.835713 -0.706520 -0.000299

12 6 0 5.180358 -0.001526 -0.190893

13 6 0 6.369355 -0.943256 -0.014203

14 1 0 -3.005202 1.117472 0.761808

15 1 0 -5.107564 -2.005146 -0.458641

16 1 0 -1.328644 -0.247296 1.967625

17 1 0 -2.950947 -0.747859 2.467595

18 1 0 -2.026823 -1.735640 1.317327

19 1 0 2.665620 0.667058 -1.214422

20 1 0 2.726611 1.076615 0.500355

21 1 0 3.795677 -1.130071 1.009856

22 1 0 3.766596 -1.547454 -0.698998

23 1 0 5.213000 0.442033 -1.191908

24 1 0 5.254785 0.832523 0.517511

25 1 0 7.320295 -0.424229 -0.166345

26 1 0 6.384129 -1.371747 0.992481

27 1 0 6.330985 -1.771779 -0.729684

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3211669 0.1932424 0.1803401

Leave Link 202 at Sat Aug 17 17:52:18 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.2437007952 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0550298920 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.1886709032 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2302

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.67D-11

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 75

GePol: Fraction of low-weight points (<1% of avg) = 3.26%

GePol: Cavity surface area = 309.646 Ang\*\*2

GePol: Cavity volume = 320.604 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057465429 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.1829243602 Hartrees.

Leave Link 301 at Sat Aug 17 17:52:18 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:52:18 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:52:18 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999842 -0.017669 -0.001119 0.001470 Ang= -2.04 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.62978204505

Leave Link 401 at Sat Aug 17 17:52:19 2019, MaxMem= 1342177280 cpu: 7.7

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 15897612.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.66D-15 for 1003.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.72D-15 for 664 455.

Iteration 1 A^-1\*A deviation from unit magnitude is 4.77D-15 for 165.

Iteration 1 A^-1\*A deviation from orthogonality is 4.93D-12 for 798 797.

E= -1658.63958854526

DIIS: error= 7.54D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.63958854526 IErMin= 1 ErrMin= 7.54D-03

ErrMax= 7.54D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.11D-02 BMatP= 8.11D-02

IDIUse=3 WtCom= 9.25D-01 WtEn= 7.54D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.430 Goal= None Shift= 0.000

Gap= 0.483 Goal= None Shift= 0.000

GapD= 0.430 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=5.75D-04 MaxDP=1.23D-02 OVMax= 4.37D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 5.75D-04 CP: 9.99D-01

E= -1658.67590127543 Delta-E= -0.036312730166 Rises=F Damp=F

DIIS: error= 8.11D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67590127543 IErMin= 2 ErrMin= 8.11D-04

ErrMax= 8.11D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.18D-03 BMatP= 8.11D-02

IDIUse=3 WtCom= 9.92D-01 WtEn= 8.11D-03

Coeff-Com: -0.671D-01 0.107D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.665D-01 0.107D+01

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=9.85D-05 MaxDP=2.06D-03 DE=-3.63D-02 OVMax= 6.22D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 8.28D-05 CP: 9.99D-01 1.09D+00

E= -1658.67620997476 Delta-E= -0.000308699337 Rises=F Damp=F

DIIS: error= 8.93D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67620997476 IErMin= 2 ErrMin= 8.11D-04

ErrMax= 8.93D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.11D-04 BMatP= 1.18D-03

IDIUse=3 WtCom= 9.91D-01 WtEn= 8.93D-03

Coeff-Com: -0.371D-01 0.506D+00 0.531D+00

Coeff-En: 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.368D-01 0.502D+00 0.535D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.131 Goal= None Shift= 0.000

RMSDP=5.74D-05 MaxDP=2.17D-03 DE=-3.09D-04 OVMax= 5.18D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 4.30D-05 CP: 9.99D-01 1.10D+00 5.49D-01

E= -1658.67630394520 Delta-E= -0.000093970438 Rises=F Damp=F

DIIS: error= 6.45D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67630394520 IErMin= 4 ErrMin= 6.45D-04

ErrMax= 6.45D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.85D-04 BMatP= 7.11D-04

IDIUse=3 WtCom= 9.94D-01 WtEn= 6.45D-03

Coeff-Com: -0.115D-01 0.141D+00 0.380D+00 0.491D+00

Coeff-En: 0.000D+00 0.000D+00 0.316D+00 0.684D+00

Coeff: -0.114D-01 0.140D+00 0.380D+00 0.492D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=2.43D-05 MaxDP=1.03D-03 DE=-9.40D-05 OVMax= 2.00D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.14D-05 CP: 9.99D-01 1.11D+00 7.25D-01 6.42D-01

E= -1658.67636343580 Delta-E= -0.000059490598 Rises=F Damp=F

DIIS: error= 6.05D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67636343580 IErMin= 5 ErrMin= 6.05D-05

ErrMax= 6.05D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.10D-06 BMatP= 2.85D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.241D-02 0.234D-01 0.125D+00 0.203D+00 0.651D+00

Coeff: -0.241D-02 0.234D-01 0.125D+00 0.203D+00 0.651D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=4.75D-06 MaxDP=2.12D-04 DE=-5.95D-05 OVMax= 4.47D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.90D-06 CP: 9.99D-01 1.11D+00 7.45D-01 6.81D-01 8.86D-01

E= -1658.67636451683 Delta-E= -0.000001081031 Rises=F Damp=F

DIIS: error= 2.94D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67636451683 IErMin= 6 ErrMin= 2.94D-05

ErrMax= 2.94D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.24D-06 BMatP= 5.10D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.592D-03-0.116D-01 0.589D-02 0.283D-01 0.357D+00 0.620D+00

Coeff: 0.592D-03-0.116D-01 0.589D-02 0.283D-01 0.357D+00 0.620D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=2.37D-06 MaxDP=8.07D-05 DE=-1.08D-06 OVMax= 2.33D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.75D-06 CP: 9.99D-01 1.11D+00 7.50D-01 7.08D-01 9.60D-01

CP: 8.57D-01

E= -1658.67636482050 Delta-E= -0.000000303668 Rises=F Damp=F

DIIS: error= 9.82D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67636482050 IErMin= 7 ErrMin= 9.82D-06

ErrMax= 9.82D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.46D-07 BMatP= 1.24D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.521D-03-0.810D-02-0.757D-02-0.392D-02 0.128D+00 0.319D+00

Coeff-Com: 0.573D+00

Coeff: 0.521D-03-0.810D-02-0.757D-02-0.392D-02 0.128D+00 0.319D+00

Coeff: 0.573D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=1.08D-06 MaxDP=4.62D-05 DE=-3.04D-07 OVMax= 9.68D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 7.42D-07 CP: 9.99D-01 1.11D+00 7.55D-01 7.05D-01 1.00D+00

CP: 9.77D-01 9.82D-01

E= -1658.67636485768 Delta-E= -0.000000037186 Rises=F Damp=F

DIIS: error= 5.89D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67636485768 IErMin= 8 ErrMin= 5.89D-06

ErrMax= 5.89D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.54D-08 BMatP= 1.46D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.147D-03-0.154D-02-0.586D-02-0.106D-01-0.200D-01 0.228D-01

Coeff-Com: 0.368D+00 0.647D+00

Coeff: 0.147D-03-0.154D-02-0.586D-02-0.106D-01-0.200D-01 0.228D-01

Coeff: 0.368D+00 0.647D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=6.38D-07 MaxDP=3.87D-05 DE=-3.72D-08 OVMax= 8.81D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 3.15D-07 CP: 9.99D-01 1.11D+00 7.55D-01 7.11D-01 1.02D+00

CP: 1.04D+00 1.18D+00 8.37D-01

E= -1658.67636487262 Delta-E= -0.000000014940 Rises=F Damp=F

DIIS: error= 1.71D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67636487262 IErMin= 9 ErrMin= 1.71D-06

ErrMax= 1.71D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.73D-09 BMatP= 4.54D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.354D-04 0.956D-03-0.143D-02-0.493D-02-0.375D-01-0.585D-01

Coeff-Com: 0.486D-01 0.327D+00 0.726D+00

Coeff: -0.354D-04 0.956D-03-0.143D-02-0.493D-02-0.375D-01-0.585D-01

Coeff: 0.486D-01 0.327D+00 0.726D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=3.22D-07 MaxDP=1.36D-05 DE=-1.49D-08 OVMax= 3.18D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.10D-07 CP: 9.99D-01 1.11D+00 7.56D-01 7.12D-01 1.03D+00

CP: 1.08D+00 1.29D+00 1.03D+00 9.07D-01

E= -1658.67636487508 Delta-E= -0.000000002460 Rises=F Damp=F

DIIS: error= 8.71D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67636487508 IErMin=10 ErrMin= 8.71D-07

ErrMax= 8.71D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.02D-09 BMatP= 6.73D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.366D-04 0.676D-03 0.116D-03-0.106D-02-0.154D-01-0.322D-01

Coeff-Com: -0.361D-01 0.687D-01 0.362D+00 0.653D+00

Coeff: -0.366D-04 0.676D-03 0.116D-03-0.106D-02-0.154D-01-0.322D-01

Coeff: -0.361D-01 0.687D-01 0.362D+00 0.653D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=9.92D-08 MaxDP=4.88D-06 DE=-2.46D-09 OVMax= 1.25D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 4.46D-08 CP: 9.99D-01 1.11D+00 7.56D-01 7.12D-01 1.03D+00

CP: 1.09D+00 1.32D+00 1.08D+00 9.96D-01 9.17D-01

E= -1658.67636487540 Delta-E= -0.000000000313 Rises=F Damp=F

DIIS: error= 2.71D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67636487540 IErMin=11 ErrMin= 2.71D-07

ErrMax= 2.71D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.06D-10 BMatP= 1.02D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.103D-04 0.147D-03 0.212D-03 0.123D-03-0.130D-02-0.548D-02

Coeff-Com: -0.224D-01-0.110D-01 0.568D-01 0.281D+00 0.702D+00

Coeff: -0.103D-04 0.147D-03 0.212D-03 0.123D-03-0.130D-02-0.548D-02

Coeff: -0.224D-01-0.110D-01 0.568D-01 0.281D+00 0.702D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=3.41D-08 MaxDP=1.72D-06 DE=-3.13D-10 OVMax= 3.65D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.74D-08 CP: 9.99D-01 1.11D+00 7.56D-01 7.12D-01 1.03D+00

CP: 1.09D+00 1.32D+00 1.09D+00 1.04D+00 1.05D+00

CP: 9.44D-01

E= -1658.67636487547 Delta-E= -0.000000000071 Rises=F Damp=F

DIIS: error= 1.14D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.67636487547 IErMin=12 ErrMin= 1.14D-07

ErrMax= 1.14D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.18D-11 BMatP= 1.06D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.376D-06-0.162D-04 0.981D-04 0.212D-03 0.153D-02 0.162D-02

Coeff-Com: -0.728D-02-0.155D-01-0.209D-01 0.581D-01 0.367D+00 0.615D+00

Coeff: -0.376D-06-0.162D-04 0.981D-04 0.212D-03 0.153D-02 0.162D-02

Coeff: -0.728D-02-0.155D-01-0.209D-01 0.581D-01 0.367D+00 0.615D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=1.10D-08 MaxDP=6.75D-07 DE=-7.14D-11 OVMax= 9.71D-07

Cycle 13 Pass 1 IDiag 1:

RMSU= 6.60D-09 CP: 9.99D-01 1.11D+00 7.56D-01 7.12D-01 1.03D+00

CP: 1.09D+00 1.33D+00 1.10D+00 1.04D+00 1.09D+00

CP: 1.05D+00 8.96D-01

E= -1658.67636487545 Delta-E= 0.000000000017 Rises=F Damp=F

DIIS: error= 3.22D-08 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=12 EnMin= -1658.67636487547 IErMin=13 ErrMin= 3.22D-08

ErrMax= 3.22D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.02D-12 BMatP= 2.18D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.159D-05-0.313D-04 0.110D-05 0.594D-04 0.856D-03 0.158D-02

Coeff-Com: 0.117D-02-0.349D-02-0.185D-01-0.286D-01 0.159D-01 0.226D+00

Coeff-Com: 0.805D+00

Coeff: 0.159D-05-0.313D-04 0.110D-05 0.594D-04 0.856D-03 0.158D-02

Coeff: 0.117D-02-0.349D-02-0.185D-01-0.286D-01 0.159D-01 0.226D+00

Coeff: 0.805D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=5.95D-09 MaxDP=2.77D-07 DE= 1.68D-11 OVMax= 7.61D-07

Error on total polarization charges = 0.04159

SCF Done: E(UB3LYP) = -1658.67636488 A.U. after 13 cycles

NFock= 13 Conv=0.60D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7551 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655249221644D+03 PE=-6.147123404015D+03 EE= 1.731014893135D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.61

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7551, after 0.7500

Leave Link 502 at Sat Aug 17 17:52:46 2019, MaxMem= 1342177280 cpu: 321.3

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 336

Leave Link 701 at Sat Aug 17 17:52:47 2019, MaxMem= 1342177280 cpu: 10.2

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:52:47 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:52:50 2019, MaxMem= 1342177280 cpu: 36.3

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.36456626D+00-2.99650736D+00 4.30445235D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000053507 -0.002882765 0.006611660

2 6 -0.000233756 0.001282730 -0.001955384

3 8 0.000544463 0.002455322 -0.002592850

4 8 0.002982834 0.001574483 -0.001163523

5 6 -0.001598865 -0.003139617 -0.000383697

6 16 -0.002483827 -0.000433479 -0.002771486

7 6 0.001654494 0.000560899 -0.000977737

8 16 0.002168655 0.000872213 -0.000131572

9 16 -0.000686458 0.000501476 0.001369072

10 6 0.000910420 0.000198783 0.002577594

11 6 -0.000012700 -0.000337606 -0.000128650

12 6 0.000253811 0.000544111 -0.001087941

13 6 0.000130396 -0.000005172 0.000250346

14 1 -0.001147054 0.000476718 -0.000176771

15 1 0.000089466 -0.000049022 0.000917016

16 1 -0.000850654 0.000552070 -0.000217780

17 1 0.000121837 -0.000071784 -0.000037103

18 1 -0.000167786 -0.000519328 0.001238087

19 1 -0.000346812 -0.000605809 -0.000733590

20 1 -0.001031613 -0.000152455 -0.000397714

21 1 -0.000695210 -0.000406376 -0.000061405

22 1 -0.000228653 -0.000415599 -0.000198971

23 1 0.000115221 0.000680341 -0.000525417

24 1 0.000368686 -0.000432700 -0.000174837

25 1 0.000036699 0.000287324 0.000261418

26 1 0.000359695 -0.000682981 0.000151938

27 1 -0.000306797 0.000148224 0.000339294

-------------------------------------------------------------------

Cartesian Forces: Max 0.006611660 RMS 0.001323719

Leave Link 716 at Sat Aug 17 17:52:50 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.005118552 RMS 0.001148356

Search for a local minimum.

Step number 49 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .11484D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43 45 44 47 46

49 48

ITU= 0 0 0 0 0 1 1 1 1 1 -1 -1 0 -1 -1 -1 0 -1 0 0

ITU= -1 -1 0 0 -1 0 0 -1 1 -1 1 -1 1 1 -1 1 -1 1 1 -1

ITU= 0 0 -1 0 0 -1 -1 0 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.97923.

Iteration 1 RMS(Cart)= 0.11452270 RMS(Int)= 0.00487039

Iteration 2 RMS(Cart)= 0.00872812 RMS(Int)= 0.00001620

Iteration 3 RMS(Cart)= 0.00004613 RMS(Int)= 0.00000242

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000242

ITry= 1 IFail=0 DXMaxC= 3.41D-01 DCOld= 1.00D+10 DXMaxT= 1.20D-01 DXLimC= 3.00D+00 Rises=T

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.84910 -0.00512 -0.01349 0.00000 -0.01349 2.83561

R2 2.28548 0.00212 0.00378 0.00000 0.00378 2.28926

R3 2.55820 -0.00187 -0.00506 0.00000 -0.00506 2.55314

R4 2.86100 0.00146 0.00412 0.00000 0.00412 2.86512

R5 3.60657 0.00182 0.00391 0.00000 0.00391 3.61048

R6 2.05690 0.00054 0.00119 0.00000 0.00119 2.05809

R7 1.83784 -0.00053 -0.00091 0.00000 -0.00091 1.83693

R8 2.06240 -0.00060 -0.00113 0.00000 -0.00113 2.06126

R9 2.06877 -0.00010 -0.00016 0.00000 -0.00016 2.06861

R10 2.06168 -0.00010 -0.00160 0.00000 -0.00160 2.06008

R11 3.30298 0.00270 0.01216 0.00000 0.01216 3.31515

R12 3.38429 0.00141 0.00340 0.00000 0.00340 3.38769

R13 3.24979 0.00103 0.00398 0.00000 0.00398 3.25377

R14 3.47809 -0.00100 -0.00579 0.00000 -0.00579 3.47231

R15 2.87983 0.00039 0.00150 0.00000 0.00150 2.88133

R16 2.06384 0.00031 0.00041 0.00000 0.00041 2.06425

R17 2.06168 -0.00046 -0.00159 0.00000 -0.00159 2.06008

R18 2.89160 0.00112 0.00252 0.00000 0.00252 2.89412

R19 2.07131 0.00019 0.00087 0.00000 0.00087 2.07218

R20 2.07020 0.00044 0.00093 0.00000 0.00093 2.07113

R21 2.88565 0.00037 0.00058 0.00000 0.00058 2.88623

R22 2.06995 0.00081 0.00194 0.00000 0.00194 2.07190

R23 2.07269 -0.00039 -0.00090 0.00000 -0.00090 2.07179

R24 2.06735 0.00015 0.00028 0.00000 0.00028 2.06763

R25 2.06771 0.00050 0.00150 0.00000 0.00150 2.06920

R26 2.06995 -0.00034 -0.00090 0.00000 -0.00090 2.06905

A1 2.17850 -0.00010 -0.00210 0.00000 -0.00210 2.17640

A2 1.98282 -0.00308 -0.00544 0.00000 -0.00544 1.97738

A3 2.12187 0.00319 0.00697 0.00000 0.00697 2.12884

A4 2.03973 -0.00336 -0.01228 0.00000 -0.01228 2.02745

A5 1.84150 -0.00097 -0.01238 0.00000 -0.01238 1.82912

A6 1.87382 0.00083 0.00005 0.00000 0.00005 1.87386

A7 1.92554 0.00367 0.02122 0.00000 0.02122 1.94676

A8 1.93843 0.00079 0.00292 0.00000 0.00292 1.94135

A9 1.83113 -0.00086 0.00061 0.00000 0.00062 1.83175

A10 1.86926 0.00024 0.00292 0.00000 0.00292 1.87218

A11 1.91995 -0.00124 -0.00688 0.00000 -0.00688 1.91307

A12 1.93337 -0.00016 -0.00693 0.00000 -0.00693 1.92644

A13 1.93726 0.00203 0.01503 0.00000 0.01503 1.95229

A14 1.88690 0.00019 -0.00344 0.00000 -0.00343 1.88347

A15 1.88861 0.00003 0.00559 0.00000 0.00559 1.89420

A16 1.89640 -0.00089 -0.00364 0.00000 -0.00364 1.89276

A17 1.79647 0.00106 0.00224 0.00000 0.00224 1.79871

A18 1.97752 0.00004 -0.00736 0.00000 -0.00735 1.97017

A19 2.14642 -0.00069 -0.00357 0.00000 -0.00356 2.14286

A20 2.15315 0.00048 0.00198 0.00000 0.00199 2.15514

A21 1.78690 0.00408 0.00854 0.00000 0.00854 1.79545

A22 1.93671 -0.00112 -0.01010 0.00000 -0.01009 1.92662

A23 1.89008 0.00004 -0.01083 0.00000 -0.01083 1.87925

A24 1.88591 -0.00019 0.00609 0.00000 0.00609 1.89200

A25 1.94436 -0.00033 -0.00504 0.00000 -0.00504 1.93932

A26 1.92318 0.00161 0.01486 0.00000 0.01486 1.93804

A27 1.88165 0.00000 0.00509 0.00000 0.00509 1.88673

A28 1.94944 0.00057 0.00350 0.00000 0.00350 1.95295

A29 1.91591 -0.00055 0.00008 0.00000 0.00008 1.91599

A30 1.92406 -0.00020 -0.00688 0.00000 -0.00688 1.91718

A31 1.90173 0.00039 0.00519 0.00000 0.00519 1.90692

A32 1.90675 -0.00016 0.00169 0.00000 0.00169 1.90844

A33 1.86383 -0.00008 -0.00382 0.00000 -0.00382 1.86001

A34 1.96675 -0.00015 -0.00069 0.00000 -0.00069 1.96606

A35 1.90348 0.00021 0.00267 0.00000 0.00267 1.90615

A36 1.90660 0.00018 0.00123 0.00000 0.00123 1.90784

A37 1.90950 0.00020 0.00330 0.00000 0.00330 1.91281

A38 1.91920 -0.00038 -0.00632 0.00000 -0.00632 1.91287

A39 1.85489 -0.00005 -0.00011 0.00000 -0.00011 1.85478

A40 1.94781 -0.00035 -0.00232 0.00000 -0.00232 1.94549

A41 1.93743 0.00090 0.00466 0.00000 0.00466 1.94210

A42 1.94294 -0.00040 -0.00014 0.00000 -0.00014 1.94281

A43 1.87759 -0.00022 -0.00063 0.00000 -0.00063 1.87695

A44 1.87388 0.00040 0.00323 0.00000 0.00323 1.87711

A45 1.88097 -0.00033 -0.00497 0.00000 -0.00497 1.87600

D1 2.65338 0.00024 0.06446 0.00000 0.06446 2.71784

D2 -1.48299 0.00204 0.07432 0.00000 0.07432 -1.40868

D3 0.46321 0.00099 0.06956 0.00000 0.06956 0.53277

D4 -0.48623 -0.00169 0.02679 0.00000 0.02679 -0.45944

D5 1.66059 0.00011 0.03665 0.00000 0.03665 1.69724

D6 -2.67640 -0.00094 0.03189 0.00000 0.03189 -2.64451

D7 -3.08770 0.00028 -0.01241 0.00000 -0.01241 -3.10011

D8 0.05581 -0.00158 -0.04891 0.00000 -0.04891 0.00690

D9 3.13839 0.00042 0.00074 0.00000 0.00074 3.13913

D10 -1.05968 -0.00024 -0.01214 0.00000 -0.01214 -1.07182

D11 1.04868 -0.00011 -0.01139 0.00000 -0.01139 1.03730

D12 1.03551 0.00120 0.00932 0.00000 0.00932 1.04483

D13 3.12063 0.00054 -0.00356 0.00000 -0.00356 3.11706

D14 -1.05420 0.00067 -0.00281 0.00000 -0.00281 -1.05700

D15 -0.98734 -0.00045 -0.00643 0.00000 -0.00643 -0.99377

D16 1.09778 -0.00111 -0.01932 0.00000 -0.01932 1.07846

D17 -3.07704 -0.00098 -0.01856 0.00000 -0.01856 -3.09560

D18 -3.10493 0.00108 0.01745 0.00000 0.01745 -3.08747

D19 -0.88694 -0.00143 0.00705 0.00000 0.00706 -0.87988

D20 1.20204 0.00091 0.02217 0.00000 0.02217 1.22421

D21 1.79712 0.00063 0.02588 0.00000 0.02588 1.82299

D22 -1.22949 0.00216 0.09049 0.00000 0.09050 -1.13899

D23 2.51919 0.00053 0.07289 0.00000 0.07289 2.59208

D24 -0.73790 -0.00109 0.00732 0.00000 0.00732 -0.73058

D25 3.12059 0.00097 0.13215 0.00000 0.13215 -3.03044

D26 -1.02340 -0.00012 0.11267 0.00000 0.11267 -0.91073

D27 1.01036 -0.00021 0.11613 0.00000 0.11613 1.12648

D28 -3.12142 -0.00050 -0.00271 0.00000 -0.00271 -3.12413

D29 -1.01004 -0.00001 0.00623 0.00000 0.00623 -1.00382

D30 1.03843 -0.00055 -0.00244 0.00000 -0.00244 1.03599

D31 1.05435 0.00044 0.02101 0.00000 0.02101 1.07536

D32 -3.11745 0.00093 0.02995 0.00000 0.02995 -3.08751

D33 -1.06898 0.00039 0.02128 0.00000 0.02128 -1.04770

D34 -1.03333 -0.00041 0.00803 0.00000 0.00803 -1.02530

D35 1.07805 0.00008 0.01697 0.00000 0.01697 1.09501

D36 3.12652 -0.00046 0.00829 0.00000 0.00829 3.13482

D37 -3.12373 -0.00030 -0.00862 0.00000 -0.00862 -3.13235

D38 -0.99967 0.00000 -0.00299 0.00000 -0.00299 -1.00266

D39 1.02082 0.00016 -0.00096 0.00000 -0.00096 1.01986

D40 1.03985 -0.00025 -0.01455 0.00000 -0.01455 1.02530

D41 -3.11928 0.00006 -0.00892 0.00000 -0.00892 -3.12820

D42 -1.09879 0.00021 -0.00689 0.00000 -0.00689 -1.10568

D43 -0.99043 -0.00028 -0.01383 0.00000 -0.01383 -1.00426

D44 1.13363 0.00002 -0.00820 0.00000 -0.00820 1.12543

D45 -3.12907 0.00018 -0.00617 0.00000 -0.00617 -3.13524

D46 3.12927 0.00017 0.00740 0.00000 0.00740 3.13667

D47 -1.05954 0.00027 0.00820 0.00000 0.00820 -1.05134

D48 1.03585 0.00018 0.00496 0.00000 0.00496 1.04081

D49 1.00863 -0.00014 0.00212 0.00000 0.00212 1.01075

D50 3.10300 -0.00004 0.00292 0.00000 0.00292 3.10592

D51 -1.08479 -0.00013 -0.00032 0.00000 -0.00032 -1.08511

D52 -1.02236 0.00002 0.00398 0.00000 0.00398 -1.01839

D53 1.07202 0.00012 0.00477 0.00000 0.00477 1.07679

D54 -3.11578 0.00003 0.00153 0.00000 0.00153 -3.11424

Item Value Threshold Converged?

Maximum Force 0.005119 0.000450 NO

RMS Force 0.001148 0.000300 NO

Maximum Displacement 0.341282 0.001800 NO

RMS Displacement 0.118158 0.001200 NO

Predicted change in Energy=-6.738714D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:52:51 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.094708 -0.406902 -0.206472

2 6 0 -2.845003 0.074196 0.470579

3 8 0 -4.887563 0.307829 -0.779263

4 8 0 -4.245123 -1.748747 -0.159545

5 6 0 -2.300411 -0.809963 1.575305

6 16 0 -1.577544 0.292471 -0.942302

7 6 0 -0.116147 0.764624 -0.094387

8 16 0 1.083002 -0.563006 0.020354

9 16 0 0.021663 2.246501 0.771479

10 6 0 2.687737 0.331745 -0.002595

11 6 0 3.846337 -0.657150 -0.070063

12 6 0 5.203641 0.052225 -0.066113

13 6 0 6.376830 -0.922417 -0.146285

14 1 0 -3.039048 1.082968 0.832318

15 1 0 -5.054516 -1.965777 -0.652178

16 1 0 -1.395394 -0.363298 1.989095

17 1 0 -3.031175 -0.901825 2.385134

18 1 0 -2.059131 -1.809565 1.213365

19 1 0 2.685310 0.994863 -0.870640

20 1 0 2.750967 0.948133 0.894341

21 1 0 3.795970 -1.346353 0.781335

22 1 0 3.759864 -1.270485 -0.974243

23 1 0 5.247940 0.751168 -0.909682

24 1 0 5.292204 0.660458 0.841729

25 1 0 7.335775 -0.395566 -0.147165

26 1 0 6.379678 -1.611559 0.704623

27 1 0 6.331005 -1.526202 -1.058502

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.500539 0.000000

3 O 1.211425 2.405981 0.000000

4 O 1.351064 2.383382 2.241938 0.000000

5 C 2.560604 1.516158 3.672439 2.770004 0.000000

6 S 2.714163 1.910584 3.314068 3.448950 2.841873

7 C 4.148974 2.870981 4.841914 4.834224 3.168312

8 S 5.185027 4.004742 6.086493 5.461434 3.731802

9 S 4.994141 3.609325 5.501250 5.918975 3.921751

10 C 6.825594 5.558906 7.615049 7.240002 5.354894

11 C 7.946159 6.752866 8.815621 8.165251 6.364990

12 C 9.310736 8.066548 10.119601 9.619323 7.729710

13 C 10.484393 9.296019 11.349041 10.654055 8.847091

14 H 2.100766 1.089096 2.571972 3.233731 2.163516

15 H 1.884137 3.209987 2.283268 0.972063 3.725946

16 H 3.479758 2.144448 4.506602 3.828456 1.090774

17 H 2.844728 2.157034 3.863011 2.943864 1.094659

18 H 2.850785 2.172068 4.056347 2.582081 1.090147

19 H 6.955193 5.764621 7.604523 7.487586 5.839302

20 H 7.064784 5.679632 7.845896 7.571599 5.391756

21 H 8.007567 6.798312 8.976388 8.105946 6.171220

22 H 7.939116 6.893471 8.792445 8.060539 6.590843

23 H 9.440376 8.237666 10.146033 9.845330 8.098759

24 H 9.505372 8.166737 10.314049 9.887741 7.768402

25 H 11.430643 10.210315 12.259866 11.659694 9.797689

26 H 10.582725 9.380367 11.525480 10.660770 8.760399

27 H 10.520184 9.439199 11.370924 10.616597 9.052694

6 7 8 9 10

6 S 0.000000

7 C 1.754301 0.000000

8 S 2.955851 1.792686 0.000000

9 S 3.051679 1.721823 3.095797 0.000000

10 C 4.367748 2.838587 1.837466 3.372452 0.000000

11 C 5.575040 4.209906 2.766416 4.875194 1.524735

12 C 6.841776 5.367351 4.167211 5.689403 2.532181

13 C 8.085893 6.708766 5.308630 7.160481 3.899099

14 H 2.431081 3.082771 4.512185 3.274975 5.835879

15 H 4.156102 5.670424 6.331602 6.748161 8.102039

16 H 3.009369 2.692504 3.171479 3.209624 4.595854

17 H 3.822462 4.174022 4.757461 4.672864 6.318932

18 H 3.049160 3.480208 3.584716 4.580026 5.347572

19 H 4.320927 2.916117 2.405871 3.370188 1.092353

20 H 4.747542 3.038354 2.414436 3.024889 1.090150

21 H 5.876336 4.530758 2.924537 5.210959 2.158411

22 H 5.561635 4.465342 2.941996 5.421336 2.158865

23 H 6.840958 5.425709 4.465280 5.690017 2.748338

24 H 7.107152 5.489755 4.459697 5.504459 2.757568

25 H 8.975127 7.541881 6.257257 7.830751 4.706818

26 H 8.345962 6.962787 5.442652 7.437301 4.231668

27 H 8.115801 6.909643 5.443639 7.575613 4.223778

11 12 13 14 15

11 C 0.000000

12 C 1.531503 0.000000

13 C 2.545500 1.527327 0.000000

14 H 7.158968 8.355330 9.676672 0.000000

15 H 9.015351 10.471179 11.490004 3.944703 0.000000

16 H 5.639347 6.924147 8.079600 2.476170 4.788886

17 H 7.306711 8.644710 9.742641 2.520060 3.801469

18 H 6.152220 7.605997 8.590758 3.077691 3.532277

19 H 2.172108 2.806746 4.222319 5.972947 8.289632

20 H 2.169526 2.782218 4.210552 5.791917 8.473969

21 H 1.096548 2.157713 2.775075 7.254080 8.987199

22 H 1.095993 2.158415 2.766799 7.418060 8.847624

23 H 2.157037 1.096401 2.158253 8.474599 10.657800

24 H 2.158236 1.096343 2.158259 8.341963 10.778843

25 H 3.500078 2.180156 1.094143 10.525322 12.499596

26 H 2.815821 2.178364 1.094974 9.797407 11.519859

27 H 2.811732 2.178811 1.094896 9.908625 11.401245

16 17 18 19 20

16 H 0.000000

17 H 1.767098 0.000000

18 H 1.770309 1.772542 0.000000

19 H 5.164768 6.846582 5.892165 0.000000

20 H 4.484490 6.251238 5.553712 1.766820 0.000000

21 H 5.419903 7.027068 5.889263 3.073090 2.523781

22 H 6.015069 7.585482 6.239947 2.509423 3.071115

23 H 7.333405 9.062668 8.028572 2.574487 3.086773

24 H 6.862106 8.608220 7.764100 3.136866 2.558009

25 H 8.988769 10.683749 9.597640 4.907498 4.889860

26 H 7.978708 9.586031 8.456449 4.787823 4.444723

27 H 8.386742 9.994943 8.696899 4.436457 4.769969

21 22 23 24 25

21 H 0.000000

22 H 1.757588 0.000000

23 H 3.060613 2.511100 0.000000

24 H 2.503928 3.061758 1.754317 0.000000

25 H 3.781049 3.773153 2.501098 2.503854 0.000000

26 H 2.598416 3.130231 3.077221 2.522590 1.765871

27 H 3.137475 2.585199 2.526182 3.077575 1.765910

26 27

26 H 0.000000

27 H 1.765861 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.60D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.103948 -0.463672 -0.130896

2 6 0 -2.848780 0.119824 0.448501

3 8 0 -4.900917 0.148767 -0.807142

4 8 0 -4.254611 -1.779370 0.136713

5 6 0 -2.295997 -0.572039 1.679148

6 16 0 -1.592277 0.101127 -0.990659

7 6 0 -0.124095 0.703467 -0.242863

8 16 0 1.075301 -0.589422 0.079025

9 16 0 0.021146 2.307087 0.367042

10 6 0 2.680220 0.286654 -0.102647

11 6 0 3.837803 -0.701916 -0.015764

12 6 0 5.195423 -0.003862 -0.138601

13 6 0 6.367502 -0.980482 -0.066699

14 1 0 -3.039533 1.174613 0.641282

15 1 0 -5.067920 -2.072883 -0.307453

16 1 0 -1.387575 -0.065104 2.007135

17 1 0 -3.020466 -0.528516 2.498617

18 1 0 -2.058007 -1.617896 1.484303

19 1 0 2.671329 0.798365 -1.067690

20 1 0 2.750726 1.041743 0.680485

21 1 0 3.793759 -1.241999 0.937540

22 1 0 3.743999 -1.455141 -0.806367

23 1 0 5.233465 0.547125 -1.085735

24 1 0 5.291343 0.744928 0.656434

25 1 0 7.326654 -0.462579 -0.161318

26 1 0 6.376668 -1.520676 0.885705

27 1 0 6.314287 -1.725675 -0.867106

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3049043 0.1933878 0.1808864

Leave Link 202 at Sat Aug 17 17:52:51 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.3384334854 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0550010737 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.2834324117 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2319

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.39D-08

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 93

GePol: Fraction of low-weight points (<1% of avg) = 4.01%

GePol: Cavity surface area = 309.183 Ang\*\*2

GePol: Cavity volume = 320.385 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057840187 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.2776483929 Hartrees.

Leave Link 301 at Sat Aug 17 17:52:51 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:52:51 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:52:51 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Lowest energy guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000418 -0.000025 0.000027 Ang= -0.05 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999850 0.017249 0.001095 -0.001443 Ang= 1.99 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 2.08D-02

Max alpha theta= 3.899 degrees.

Max beta theta= 3.940 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 17:52:51 2019, MaxMem= 1342177280 cpu: 4.3

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16133283.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.00D-15 for 2319.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.34D-15 for 2286 49.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.55D-15 for 2319.

Iteration 1 A^-1\*A deviation from orthogonality is 2.65D-09 for 912 739.

Iteration 2 A\*A^-1 deviation from unit magnitude is 3.55D-15 for 542.

Iteration 2 A\*A^-1 deviation from orthogonality is 2.83D-15 for 2292 401.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 2209.

Iteration 2 A^-1\*A deviation from orthogonality is 4.71D-16 for 2295 2274.

E= -1658.67701662643

DIIS: error= 1.70D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67701662643 IErMin= 1 ErrMin= 1.70D-05

ErrMax= 1.70D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.52D-07 BMatP= 2.52D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 88.714 Goal= None Shift= 0.000

Gap= 88.711 Goal= None Shift= 0.000

RMSDP=9.83D-07 MaxDP=4.61D-05 OVMax= 6.45D-05

Cycle 2 Pass 1 IDiag 1:

RMSU= 9.81D-07 CP: 1.00D+00

E= -1658.67701666032 Delta-E= -0.000000033889 Rises=F Damp=F

DIIS: error= 1.38D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67701666032 IErMin= 2 ErrMin= 1.38D-05

ErrMax= 1.38D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.88D-07 BMatP= 2.52D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.450D+00 0.550D+00

Coeff: 0.450D+00 0.550D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=7.16D-07 MaxDP=4.55D-05 DE=-3.39D-08 OVMax= 5.86D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 5.80D-07 CP: 1.00D+00 5.75D-01

E= -1658.67701668142 Delta-E= -0.000000021097 Rises=F Damp=F

DIIS: error= 8.77D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67701668142 IErMin= 3 ErrMin= 8.77D-06

ErrMax= 8.77D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.28D-08 BMatP= 1.88D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.851D-02 0.380D+00 0.612D+00

Coeff: 0.851D-02 0.380D+00 0.612D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.28D-07 MaxDP=1.88D-05 DE=-2.11D-08 OVMax= 3.62D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.50D-07 CP: 1.00D+00 7.54D-01 6.00D-01

E= -1658.67701669316 Delta-E= -0.000000011747 Rises=F Damp=F

DIIS: error= 3.85D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67701669316 IErMin= 4 ErrMin= 3.85D-06

ErrMax= 3.85D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.10D-09 BMatP= 7.28D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.177D-01 0.213D+00 0.390D+00 0.415D+00

Coeff: -0.177D-01 0.213D+00 0.390D+00 0.415D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=9.33D-08 MaxDP=4.41D-06 DE=-1.17D-08 OVMax= 1.04D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.72D-08 CP: 1.00D+00 7.54D-01 6.56D-01 4.74D-01

E= -1658.67701669444 Delta-E= -0.000000001279 Rises=F Damp=F

DIIS: error= 4.55D-07 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67701669444 IErMin= 5 ErrMin= 4.55D-07

ErrMax= 4.55D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.60D-10 BMatP= 7.10D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.872D-02 0.764D-01 0.145D+00 0.198D+00 0.589D+00

Coeff: -0.872D-02 0.764D-01 0.145D+00 0.198D+00 0.589D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.69D-08 MaxDP=1.08D-06 DE=-1.28D-09 OVMax= 1.25D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.44D-08 CP: 1.00D+00 7.57D-01 6.58D-01 4.95D-01 7.98D-01

E= -1658.67701669447 Delta-E= -0.000000000029 Rises=F Damp=F

DIIS: error= 8.61D-08 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67701669447 IErMin= 6 ErrMin= 8.61D-08

ErrMax= 8.61D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.31D-11 BMatP= 1.60D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.239D-02 0.171D-01 0.345D-01 0.564D-01 0.279D+00 0.615D+00

Coeff: -0.239D-02 0.171D-01 0.345D-01 0.564D-01 0.279D+00 0.615D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.30D-09 MaxDP=3.16D-07 DE=-2.91D-11 OVMax= 6.57D-07

Error on total polarization charges = 0.04162

SCF Done: E(UB3LYP) = -1658.67701669 A.U. after 6 cycles

NFock= 6 Conv=0.63D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655236605652D+03 PE=-6.147321681225D+03 EE= 1.731130410486D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.63

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:53:06 2019, MaxMem= 1342177280 cpu: 172.3

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 335

Leave Link 701 at Sat Aug 17 17:53:08 2019, MaxMem= 1342177280 cpu: 10.3

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:53:08 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:53:11 2019, MaxMem= 1342177280 cpu: 38.3

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.40689257D+00-2.94462813D+00 6.36028801D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000011134 -0.000037953 0.000081813

2 6 0.000022160 -0.000025686 0.000024510

3 8 -0.000045738 0.000134925 -0.000010272

4 8 0.000054357 -0.000038501 -0.000036524

5 6 -0.000023824 -0.000052619 0.000010979

6 16 0.000055600 0.000047214 -0.000018874

7 6 -0.000025774 0.000007555 0.000015872

8 16 0.000013078 0.000022886 -0.000008113

9 16 -0.000018453 -0.000029209 0.000068797

10 6 0.000031464 -0.000000073 0.000046429

11 6 -0.000005323 0.000008029 -0.000011225

12 6 -0.000000894 0.000007407 -0.000021220

13 6 -0.000002139 0.000015234 -0.000012400

14 1 -0.000025812 -0.000001865 0.000042831

15 1 -0.000015397 0.000027258 -0.000036251

16 1 0.000005128 -0.000026673 -0.000005229

17 1 0.000002800 -0.000047345 -0.000006912

18 1 0.000005300 -0.000022729 -0.000042296

19 1 0.000016918 0.000024184 0.000011367

20 1 -0.000036150 -0.000025056 0.000035021

21 1 0.000001133 -0.000024017 -0.000030432

22 1 -0.000007699 0.000007902 -0.000036603

23 1 0.000005536 0.000038316 0.000008861

24 1 0.000004348 -0.000018754 0.000023383

25 1 0.000007279 0.000010764 -0.000009780

26 1 -0.000001463 -0.000032587 -0.000039405

27 1 -0.000005300 0.000031394 -0.000044329

-------------------------------------------------------------------

Cartesian Forces: Max 0.000134925 RMS 0.000031994

Leave Link 716 at Sat Aug 17 17:53:11 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000108143 RMS 0.000021544

Search for a local minimum.

Step number 50 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .21544D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43 45 44 47 46

49 48 50

ITU= 0 0 0 0 0 0 1 1 1 1 1 -1 -1 0 -1 -1 -1 0 -1 0

ITU= 0 -1 -1 0 0 -1 0 0 -1 1 -1 1 -1 1 1 -1 1 -1 1 1

ITU= -1 0 0 -1 0 0 -1 -1 0 0

Use linear search instead of GDIIS.

Eigenvalues --- -0.00555 0.00000 0.00000 0.00032 0.00248

Eigenvalues --- 0.00289 0.00324 0.00470 0.00761 0.01957

Eigenvalues --- 0.02489 0.03232 0.03403 0.03501 0.03922

Eigenvalues --- 0.04290 0.04741 0.04815 0.05035 0.05263

Eigenvalues --- 0.05448 0.05474 0.05576 0.05790 0.06679

Eigenvalues --- 0.08198 0.08323 0.10762 0.11323 0.11689

Eigenvalues --- 0.12408 0.13409 0.14342 0.15348 0.15762

Eigenvalues --- 0.15959 0.16086 0.16223 0.16592 0.17898

Eigenvalues --- 0.18680 0.19466 0.19677 0.21782 0.22173

Eigenvalues --- 0.22419 0.23509 0.24068 0.24913 0.26270

Eigenvalues --- 0.26929 0.28419 0.29210 0.29322 0.29585

Eigenvalues --- 0.29913 0.30798 0.33210 0.33515 0.33861

Eigenvalues --- 0.33878 0.33923 0.33977 0.34015 0.34076

Eigenvalues --- 0.34085 0.34151 0.34202 0.34560 0.34800

Eigenvalues --- 0.35344 0.35441 0.47774 0.52545 0.89753

Eigenvalue 1 is -5.55D-03 should be greater than 0.000000 Eigenvector:

D24 D23 D5 D8 D22

1 -0.38333 -0.28382 0.27802 0.24451 0.23666

D4 D26 D16 D27 A9

1 0.21937 0.21467 0.20278 0.17601 -0.17506

RFO step: Lambda=-5.54763441D-03 EMin=-5.54727381D-03

I= 1 Eig= -5.55D-03 Dot1= -1.34D-05

I= 1 Stepn= -2.99D-01 RXN= 2.99D-01 EDone=F

Mixed 1 eigenvectors in step. Raw Step.Grad= 1.34D-05.

RFO eigenvector is Hessian eigenvector with negative curvature.

Taking step of 2.99D-01 in eigenvector direction(s). Step.Grad= -3.16D-06.

Quartic linear search produced a step of 0.00462.

Iteration 1 RMS(Cart)= 0.08294072 RMS(Int)= 0.00252529

Iteration 2 RMS(Cart)= 0.00425927 RMS(Int)= 0.00008902

Iteration 3 RMS(Cart)= 0.00001345 RMS(Int)= 0.00008873

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00008873

ITry= 1 IFail=0 DXMaxC= 2.96D-01 DCOld= 1.00D+10 DXMaxT= 1.20D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83561 -0.00001 0.00000 0.01603 0.01603 2.85164

R2 2.28926 0.00011 0.00000 0.00747 0.00747 2.29673

R3 2.55314 0.00004 0.00000 0.00358 0.00358 2.55672

R4 2.86512 -0.00001 0.00000 -0.00641 -0.00641 2.85872

R5 3.61048 0.00006 0.00000 0.02727 0.02727 3.63775

R6 2.05809 0.00002 0.00000 -0.00350 -0.00350 2.05459

R7 1.83693 0.00001 0.00000 -0.00011 -0.00011 1.83682

R8 2.06126 0.00001 0.00000 -0.00341 -0.00341 2.05785

R9 2.06861 0.00000 0.00000 0.00266 0.00266 2.07127

R10 2.06008 0.00000 0.00000 -0.00453 -0.00453 2.05555

R11 3.31515 -0.00003 0.00000 0.00125 0.00125 3.31640

R12 3.38769 0.00002 0.00000 -0.00497 -0.00497 3.38272

R13 3.25377 -0.00001 0.00000 0.01254 0.01254 3.26631

R14 3.47231 0.00000 0.00000 -0.00315 -0.00315 3.46916

R15 2.88133 0.00001 0.00000 0.00505 0.00505 2.88638

R16 2.06425 0.00001 0.00000 0.00164 0.00164 2.06589

R17 2.06008 0.00000 0.00000 -0.00135 -0.00135 2.05873

R18 2.89412 0.00002 0.00000 0.00117 0.00117 2.89529

R19 2.07218 0.00001 0.00000 0.00364 0.00364 2.07582

R20 2.07113 0.00002 0.00000 0.00137 0.00137 2.07249

R21 2.88623 0.00000 0.00000 -0.00062 -0.00062 2.88560

R22 2.07190 0.00002 0.00000 0.00203 0.00203 2.07393

R23 2.07179 0.00000 0.00000 0.00148 0.00148 2.07327

R24 2.06763 0.00001 0.00000 0.00214 0.00214 2.06977

R25 2.06920 0.00001 0.00000 0.00400 0.00400 2.07320

R26 2.06905 0.00000 0.00000 0.00169 0.00169 2.07074

A1 2.17640 -0.00005 0.00000 -0.01894 -0.01919 2.15721

A2 1.97738 -0.00002 0.00000 0.01752 0.01726 1.99464

A3 2.12884 0.00007 0.00000 0.00009 -0.00018 2.12866

A4 2.02745 0.00000 0.00000 0.00460 0.00448 2.03192

A5 1.82912 0.00002 0.00000 -0.01281 -0.01281 1.81631

A6 1.87386 -0.00002 0.00000 -0.01012 -0.01019 1.86367

A7 1.94676 -0.00002 0.00000 -0.00833 -0.00833 1.93843

A8 1.94135 0.00000 0.00000 -0.01999 -0.02006 1.92129

A9 1.83175 0.00001 0.00000 0.05238 0.05248 1.88422

A10 1.87218 -0.00001 0.00000 0.02237 0.02237 1.89455

A11 1.91307 -0.00003 0.00000 -0.02182 -0.02193 1.89115

A12 1.92644 0.00000 0.00000 -0.01070 -0.01084 1.91560

A13 1.95229 0.00000 0.00000 0.01415 0.01421 1.96649

A14 1.88347 0.00001 0.00000 -0.00157 -0.00189 1.88158

A15 1.89420 0.00001 0.00000 0.01148 0.01157 1.90577

A16 1.89276 0.00001 0.00000 0.00860 0.00862 1.90138

A17 1.79871 -0.00008 0.00000 0.01321 0.01321 1.81192

A18 1.97017 0.00001 0.00000 -0.00368 -0.00381 1.96636

A19 2.14286 -0.00003 0.00000 0.01051 0.01039 2.15324

A20 2.15514 0.00002 0.00000 -0.00202 -0.00215 2.15299

A21 1.79545 0.00009 0.00000 0.01584 0.01584 1.81128

A22 1.92662 0.00000 0.00000 -0.01583 -0.01600 1.91062

A23 1.87925 0.00001 0.00000 -0.01799 -0.01828 1.86097

A24 1.89200 -0.00003 0.00000 0.01546 0.01554 1.90754

A25 1.93932 -0.00002 0.00000 -0.00640 -0.00670 1.93263

A26 1.93804 0.00003 0.00000 0.01378 0.01381 1.95185

A27 1.88673 0.00001 0.00000 0.01109 0.01113 1.89786

A28 1.95295 -0.00001 0.00000 0.00602 0.00598 1.95892

A29 1.91599 0.00000 0.00000 0.00800 0.00793 1.92392

A30 1.91718 0.00001 0.00000 -0.01519 -0.01517 1.90202

A31 1.90692 0.00000 0.00000 0.00482 0.00473 1.91165

A32 1.90844 0.00000 0.00000 0.00231 0.00233 1.91076

A33 1.86001 -0.00001 0.00000 -0.00650 -0.00648 1.85352

A34 1.96606 0.00000 0.00000 -0.00137 -0.00137 1.96468

A35 1.90615 0.00001 0.00000 -0.00133 -0.00134 1.90481

A36 1.90784 0.00000 0.00000 0.00520 0.00519 1.91303

A37 1.91281 0.00000 0.00000 0.00150 0.00150 1.91431

A38 1.91287 0.00000 0.00000 -0.00599 -0.00599 1.90689

A39 1.85478 0.00000 0.00000 0.00224 0.00224 1.85701

A40 1.94549 0.00000 0.00000 0.00531 0.00529 1.95078

A41 1.94210 0.00001 0.00000 0.00199 0.00199 1.94409

A42 1.94281 -0.00001 0.00000 0.00397 0.00396 1.94676

A43 1.87695 0.00000 0.00000 -0.00402 -0.00403 1.87293

A44 1.87711 0.00000 0.00000 0.00087 0.00084 1.87795

A45 1.87600 0.00000 0.00000 -0.00889 -0.00889 1.86711

D1 2.71784 -0.00001 -0.00001 -0.02391 -0.02398 2.69386

D2 -1.40868 -0.00001 -0.00001 -0.04146 -0.04153 -1.45021

D3 0.53277 0.00000 -0.00001 0.00767 0.00759 0.54036

D4 -0.45944 -0.00003 0.00000 -0.06563 -0.06557 -0.52500

D5 1.69724 -0.00003 0.00000 -0.08318 -0.08311 1.61412

D6 -2.64451 -0.00001 0.00000 -0.03406 -0.03400 -2.67850

D7 -3.10011 0.00000 0.00000 -0.03226 -0.03207 -3.13218

D8 0.00690 -0.00001 0.00000 -0.07316 -0.07334 -0.06644

D9 3.13913 0.00001 0.00000 -0.01171 -0.01185 3.12727

D10 -1.07182 0.00001 0.00000 -0.03367 -0.03361 -1.10543

D11 1.03730 0.00002 0.00000 -0.02061 -0.02062 1.01667

D12 1.04483 0.00000 0.00000 0.00864 0.00850 1.05332

D13 3.11706 -0.00001 0.00000 -0.01333 -0.01326 3.10381

D14 -1.05700 0.00000 0.00000 -0.00027 -0.00027 -1.05728

D15 -0.99377 -0.00001 0.00000 -0.03871 -0.03876 -1.03253

D16 1.07846 -0.00001 0.00000 -0.06067 -0.06051 1.01795

D17 -3.09560 0.00000 0.00000 -0.04761 -0.04753 3.14005

D18 -3.08747 0.00001 0.00000 -0.01845 -0.01856 -3.10603

D19 -0.87988 0.00001 0.00000 -0.02669 -0.02669 -0.90657

D20 1.22421 0.00001 0.00000 -0.02302 -0.02293 1.20129

D21 1.82299 -0.00003 0.00000 -0.04275 -0.04269 1.78031

D22 -1.13899 0.00002 -0.00001 -0.07081 -0.07088 -1.20987

D23 2.59208 0.00004 -0.00001 0.08492 0.08496 2.67704

D24 -0.73058 -0.00002 0.00000 0.11469 0.11464 -0.61594

D25 -3.03044 0.00000 -0.00001 -0.03554 -0.03572 -3.06616

D26 -0.91073 -0.00002 -0.00001 -0.06423 -0.06403 -0.97476

D27 1.12648 -0.00002 -0.00001 -0.05266 -0.05271 1.07377

D28 -3.12413 0.00000 0.00000 -0.04163 -0.04157 3.11748

D29 -1.00382 0.00000 0.00000 -0.02596 -0.02587 -1.02968

D30 1.03599 0.00000 0.00000 -0.03806 -0.03798 0.99801

D31 1.07536 0.00000 0.00000 -0.00468 -0.00476 1.07061

D32 -3.08751 0.00000 0.00000 0.01099 0.01095 -3.07656

D33 -1.04770 0.00000 0.00000 -0.00111 -0.00117 -1.04887

D34 -1.02530 -0.00001 0.00000 -0.02368 -0.02372 -1.04902

D35 1.09501 -0.00001 0.00000 -0.00801 -0.00801 1.08700

D36 3.13482 -0.00001 0.00000 -0.02011 -0.02013 3.11469

D37 -3.13235 -0.00001 0.00000 -0.01814 -0.01813 3.13271

D38 -1.00266 0.00000 0.00000 -0.01809 -0.01808 -1.02075

D39 1.01986 0.00000 0.00000 -0.01326 -0.01325 1.00661

D40 1.02530 -0.00001 0.00000 -0.03555 -0.03556 0.98974

D41 -3.12820 0.00000 0.00000 -0.03550 -0.03551 3.11947

D42 -1.10568 0.00000 0.00000 -0.03067 -0.03068 -1.13635

D43 -1.00426 0.00000 0.00000 -0.03176 -0.03176 -1.03602

D44 1.12543 0.00000 0.00000 -0.03172 -0.03172 1.09371

D45 -3.13524 0.00000 0.00000 -0.02689 -0.02688 3.12107

D46 3.13667 0.00001 0.00000 -0.00542 -0.00542 3.13125

D47 -1.05134 0.00001 0.00000 -0.00558 -0.00558 -1.05692

D48 1.04081 0.00001 0.00000 -0.01283 -0.01284 1.02797

D49 1.01075 0.00000 0.00000 -0.00385 -0.00384 1.00690

D50 3.10592 0.00000 0.00000 -0.00401 -0.00401 3.10192

D51 -1.08511 0.00000 0.00000 -0.01126 -0.01127 -1.09638

D52 -1.01839 0.00000 0.00000 -0.00398 -0.00397 -1.02236

D53 1.07679 0.00000 0.00000 -0.00414 -0.00413 1.07266

D54 -3.11424 0.00000 0.00000 -0.01139 -0.01140 -3.12564

Item Value Threshold Converged?

Maximum Force 0.000108 0.000450 YES

RMS Force 0.000022 0.000300 YES

Maximum Displacement 0.295827 0.001800 NO

RMS Displacement 0.084852 0.001200 NO

Predicted change in Energy=-2.616947D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:53:11 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.107544 -0.420180 -0.142559

2 6 0 -2.837284 0.055264 0.518908

3 8 0 -4.936455 0.327814 -0.622718

4 8 0 -4.211725 -1.765217 -0.245109

5 6 0 -2.231296 -0.866973 1.553667

6 16 0 -1.624321 0.340893 -0.948342

7 6 0 -0.132129 0.835608 -0.168271

8 16 0 1.072675 -0.485574 -0.083257

9 16 0 0.061574 2.351858 0.638593

10 6 0 2.683305 0.393958 -0.033776

11 6 0 3.820909 -0.624705 -0.067708

12 6 0 5.199025 0.044747 -0.063083

13 6 0 6.342255 -0.967325 -0.084370

14 1 0 -3.058218 1.022175 0.964294

15 1 0 -5.050570 -1.977529 -0.687894

16 1 0 -1.320239 -0.406020 1.932278

17 1 0 -2.922789 -0.983952 2.395995

18 1 0 -1.994579 -1.849770 1.152074

19 1 0 2.714808 1.038781 -0.916016

20 1 0 2.725155 1.018497 0.857890

21 1 0 3.742736 -1.310100 0.787145

22 1 0 3.718264 -1.244149 -0.966897

23 1 0 5.278531 0.710515 -0.931924

24 1 0 5.296027 0.681566 0.825026

25 1 0 7.320608 -0.474975 -0.091332

26 1 0 6.312853 -1.622680 0.794979

27 1 0 6.290585 -1.614164 -0.967369

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.509022 0.000000

3 O 1.215377 2.405019 0.000000

4 O 1.352958 2.405611 2.246909 0.000000

5 C 2.568484 1.512768 3.671792 2.822152 0.000000

6 S 2.719359 1.925016 3.328128 3.409530 2.843837

7 C 4.169123 2.898105 4.852414 4.838729 3.204739

8 S 5.180971 3.992854 6.087878 5.439537 3.706913

9 S 5.067143 3.700276 5.537866 5.999361 4.056536

10 C 6.840343 5.558514 7.642773 7.228288 5.316317

11 C 7.931444 6.718483 8.826481 8.115138 6.270306

12 C 9.318514 8.057362 10.154865 9.584953 7.658642

13 C 10.464275 9.256001 11.365584 10.585318 8.729205

14 H 2.099189 1.087242 2.555096 3.250044 2.144770

15 H 1.900533 3.238404 2.309086 0.972006 3.769116

16 H 3.474797 2.124105 4.488155 3.866410 1.088967

17 H 2.857575 2.147263 3.858524 3.040915 1.096067

18 H 2.860843 2.177202 4.067726 2.622024 1.087751

19 H 7.019351 5.818250 7.689820 7.502625 5.847664

20 H 7.053826 5.655391 7.833870 7.555526 5.348412

21 H 7.955074 6.725536 8.944207 8.034061 6.039286

22 H 7.912125 6.846262 8.803050 7.979801 6.472463

23 H 9.486832 8.270473 10.226829 9.831884 8.066234

24 H 9.517205 8.163130 10.340444 9.875691 7.719422

25 H 11.428398 10.190010 12.294814 11.605304 9.700441

26 H 10.531365 9.306810 11.504835 10.576807 8.610992

27 H 10.498904 9.397552 11.398969 10.528200 8.918317

6 7 8 9 10

6 S 0.000000

7 C 1.754962 0.000000

8 S 2.950459 1.790056 0.000000

9 S 3.066690 1.728458 3.097485 0.000000

10 C 4.403963 2.853036 1.835798 3.340499 0.000000

11 C 5.599860 4.215346 2.751798 4.846792 1.527406

12 C 6.886904 5.390523 4.160339 5.675255 2.540011

13 C 8.119373 6.721254 5.291556 7.140490 3.904300

14 H 2.485635 3.143169 4.520503 3.406941 5.861390

15 H 4.145129 5.689887 6.331323 6.829142 8.115704

16 H 2.991373 2.713954 3.129655 3.344984 4.531412

17 H 3.824372 4.204050 4.728509 4.808588 6.263443

18 H 3.057424 3.524668 3.577027 4.705859 5.321951

19 H 4.395012 2.950500 2.390344 3.343745 1.093223

20 H 4.758105 3.041468 2.424598 2.986739 1.089435

21 H 5.877329 4.531166 2.926887 5.194513 2.167975

22 H 5.572784 4.448452 2.890571 5.374035 2.150639

23 H 6.912761 5.465717 4.454222 5.690094 2.764431

24 H 7.152070 5.520439 4.474806 5.497647 2.765243

25 H 9.022852 7.567486 6.247947 7.824152 4.718361

26 H 8.360234 6.964827 5.433578 7.409446 4.234061

27 H 8.152812 6.920346 5.411280 7.557051 4.232802

11 12 13 14 15

11 C 0.000000

12 C 1.532120 0.000000

13 C 2.544572 1.526996 0.000000

14 H 7.148401 8.378123 9.665749 0.000000

15 H 8.995438 10.465859 11.453437 3.961996 0.000000

16 H 5.520794 6.832676 7.943283 2.448940 4.821858

17 H 7.188627 8.548050 9.591326 2.468330 3.876211

18 H 6.067006 7.537490 8.474096 3.068331 3.569438

19 H 2.170316 2.808368 4.227820 6.071546 8.333742

20 H 2.181175 2.813612 4.232582 5.784353 8.475112

21 H 1.098477 2.163164 2.763066 7.191931 8.941109

22 H 1.096717 2.161201 2.782232 7.401786 8.803871

23 H 2.157393 1.097475 2.159861 8.555359 10.675930

24 H 2.163166 1.097126 2.154167 8.362345 10.789429

25 H 3.502980 2.184496 1.095277 10.539252 12.476362

26 H 2.819568 2.181099 1.097091 9.738629 11.465261

27 H 2.808507 2.182022 1.095791 9.903622 11.350416

16 17 18 19 20

16 H 0.000000

17 H 1.765562 0.000000

18 H 1.774223 1.777232 0.000000

19 H 5.146050 6.844221 5.899072 0.000000

20 H 4.421399 6.186667 5.530767 1.774052 0.000000

21 H 5.269004 6.864692 5.774184 3.078089 2.542212

22 H 5.873175 7.448512 6.123185 2.494250 3.071756

23 H 7.279702 9.011544 7.987255 2.584703 3.133372

24 H 6.795867 8.531754 7.724477 3.133930 2.593064

25 H 8.874907 10.553343 9.497833 4.917820 4.924395

26 H 7.812669 9.395122 8.318204 4.791325 4.455485

27 H 8.233602 9.828308 8.555203 4.452744 4.793200

21 22 23 24 25

21 H 0.000000

22 H 1.755452 0.000000

23 H 3.065412 2.501274 0.000000

24 H 2.526040 3.067361 1.757275 0.000000

25 H 3.777608 3.786176 2.506403 2.505240 0.000000

26 H 2.589067 3.159016 3.081527 2.518806 1.765883

27 H 3.108425 2.598797 2.535673 3.077694 1.768090

26 27

26 H 0.000000

27 H 1.762509 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 8.14D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.112885 -0.482879 -0.071258

2 6 0 -2.837326 0.057490 0.527155

3 8 0 -4.943709 0.211469 -0.623302

4 8 0 -4.220140 -1.830901 -0.028515

5 6 0 -2.225965 -0.750170 1.650718

6 16 0 -1.633843 0.181375 -0.970165

7 6 0 -0.135519 0.753050 -0.257350

8 16 0 1.067493 -0.554428 -0.039261

9 16 0 0.066338 2.346482 0.381237

10 6 0 2.679977 0.321338 -0.094801

11 6 0 3.815520 -0.697929 -0.026924

12 6 0 5.194818 -0.035257 -0.103043

13 6 0 6.336084 -1.046631 -0.023336

14 1 0 -3.053521 1.067072 0.867888

15 1 0 -5.062345 -2.087311 -0.440511

16 1 0 -1.311545 -0.253599 1.971814

17 1 0 -2.911933 -0.774578 2.505244

18 1 0 -1.993718 -1.770899 1.355122

19 1 0 2.706634 0.867922 -1.041201

20 1 0 2.728981 1.037643 0.724573

21 1 0 3.741935 -1.287667 0.896896

22 1 0 3.705679 -1.409822 -0.853925

23 1 0 5.269606 0.533466 -1.038677

24 1 0 5.298970 0.692739 0.711119

25 1 0 7.315237 -0.560291 -0.089390

26 1 0 6.311489 -1.604001 0.921303

27 1 0 6.277278 -1.784156 -0.831641

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2739592 0.1943907 0.1803643

Leave Link 202 at Sat Aug 17 17:53:11 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1100.3159146578 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0547277809 Hartrees.

Nuclear repulsion after empirical dispersion term = 1100.2611868769 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2334

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.54D-09

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 79

GePol: Fraction of low-weight points (<1% of avg) = 3.38%

GePol: Cavity surface area = 309.464 Ang\*\*2

GePol: Cavity volume = 320.754 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057446456 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1100.2554422312 Hartrees.

Leave Link 301 at Sat Aug 17 17:53:11 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.87D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:53:11 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:53:11 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999743 -0.022588 -0.001598 0.000769 Ang= -2.60 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.62931319501

Leave Link 401 at Sat Aug 17 17:53:12 2019, MaxMem= 1342177280 cpu: 7.6

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16342668.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.22D-15 for 2324.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.08D-15 for 2300 73.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.11D-15 for 2324.

Iteration 1 A^-1\*A deviation from orthogonality is 5.38D-12 for 817 810.

E= -1658.65408617721

DIIS: error= 4.48D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.65408617721 IErMin= 1 ErrMin= 4.48D-03

ErrMax= 4.48D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.91D-02 BMatP= 4.91D-02

IDIUse=3 WtCom= 9.55D-01 WtEn= 4.48D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.428 Goal= None Shift= 0.000

Gap= 0.484 Goal= None Shift= 0.000

GapD= 0.428 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=5.28D-04 MaxDP=1.51D-02 OVMax= 3.32D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 5.28D-04 CP: 9.99D-01

E= -1658.67555226394 Delta-E= -0.021466086729 Rises=F Damp=F

DIIS: error= 9.54D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67555226394 IErMin= 2 ErrMin= 9.54D-04

ErrMax= 9.54D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.13D-03 BMatP= 4.91D-02

IDIUse=3 WtCom= 9.90D-01 WtEn= 9.54D-03

Coeff-Com: -0.561D-01 0.106D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.556D-01 0.106D+01

Gap= 0.119 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.02D-04 MaxDP=2.68D-03 DE=-2.15D-02 OVMax= 7.56D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 9.53D-05 CP: 9.99D-01 1.07D+00

E= -1658.67567500532 Delta-E= -0.000122741385 Rises=F Damp=F

DIIS: error= 1.21D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67567500532 IErMin= 2 ErrMin= 9.54D-04

ErrMax= 1.21D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.24D-03 BMatP= 1.13D-03

IDIUse=3 WtCom= 9.88D-01 WtEn= 1.21D-02

Coeff-Com: -0.416D-01 0.571D+00 0.471D+00

Coeff-En: 0.000D+00 0.313D+00 0.687D+00

Coeff: -0.411D-01 0.568D+00 0.473D+00

Gap= 0.119 Goal= None Shift= 0.000

Gap= 0.134 Goal= None Shift= 0.000

RMSDP=6.20D-05 MaxDP=3.50D-03 DE=-1.23D-04 OVMax= 6.12D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 4.72D-05 CP: 9.99D-01 1.10D+00 6.03D-01

E= -1658.67587172610 Delta-E= -0.000196720783 Rises=F Damp=F

DIIS: error= 5.88D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67587172610 IErMin= 4 ErrMin= 5.88D-04

ErrMax= 5.88D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.60D-04 BMatP= 1.13D-03

IDIUse=3 WtCom= 9.94D-01 WtEn= 5.88D-03

Coeff-Com: -0.140D-01 0.174D+00 0.317D+00 0.523D+00

Coeff-En: 0.000D+00 0.000D+00 0.194D+00 0.806D+00

Coeff: -0.139D-01 0.173D+00 0.317D+00 0.524D+00

Gap= 0.119 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.23D-05 MaxDP=9.56D-04 DE=-1.97D-04 OVMax= 2.31D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.47D-05 CP: 9.99D-01 1.10D+00 6.97D-01 7.10D-01

E= -1658.67592142648 Delta-E= -0.000049700378 Rises=F Damp=F

DIIS: error= 9.56D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67592142648 IErMin= 5 ErrMin= 9.56D-05

ErrMax= 9.56D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.77D-06 BMatP= 2.60D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.334D-02 0.373D-01 0.117D+00 0.252D+00 0.597D+00

Coeff: -0.334D-02 0.373D-01 0.117D+00 0.252D+00 0.597D+00

Gap= 0.119 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.56D-06 MaxDP=2.33D-04 DE=-4.97D-05 OVMax= 8.03D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 4.34D-06 CP: 9.99D-01 1.10D+00 7.24D-01 7.86D-01 8.76D-01

E= -1658.67592370512 Delta-E= -0.000002278634 Rises=F Damp=F

DIIS: error= 2.79D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67592370512 IErMin= 6 ErrMin= 2.79D-05

ErrMax= 2.79D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.19D-06 BMatP= 9.77D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.770D-03-0.149D-01-0.428D-03 0.254D-01 0.271D+00 0.718D+00

Coeff: 0.770D-03-0.149D-01-0.428D-03 0.254D-01 0.271D+00 0.718D+00

Gap= 0.119 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.23D-06 MaxDP=1.20D-04 DE=-2.28D-06 OVMax= 3.82D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.97D-06 CP: 9.99D-01 1.11D+00 7.39D-01 8.24D-01 9.49D-01

CP: 1.03D+00

E= -1658.67592404608 Delta-E= -0.000000340961 Rises=F Damp=F

DIIS: error= 1.28D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67592404608 IErMin= 7 ErrMin= 1.28D-05

ErrMax= 1.28D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.05D-07 BMatP= 1.19D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.809D-03-0.124D-01-0.145D-01-0.182D-01 0.679D-01 0.360D+00

Coeff-Com: 0.616D+00

Coeff: 0.809D-03-0.124D-01-0.145D-01-0.182D-01 0.679D-01 0.360D+00

Coeff: 0.616D+00

Gap= 0.119 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.32D-06 MaxDP=5.08D-05 DE=-3.41D-07 OVMax= 1.65D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 8.13D-07 CP: 9.99D-01 1.11D+00 7.42D-01 8.31D-01 9.96D-01

CP: 1.15D+00 9.70D-01

E= -1658.67592410471 Delta-E= -0.000000058630 Rises=F Damp=F

DIIS: error= 7.42D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67592410471 IErMin= 8 ErrMin= 7.42D-06

ErrMax= 7.42D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.41D-08 BMatP= 2.05D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.274D-03-0.346D-02-0.746D-02-0.147D-01-0.132D-01 0.585D-01

Coeff-Com: 0.360D+00 0.620D+00

Coeff: 0.274D-03-0.346D-02-0.746D-02-0.147D-01-0.132D-01 0.585D-01

Coeff: 0.360D+00 0.620D+00

Gap= 0.119 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=8.58D-07 MaxDP=3.38D-05 DE=-5.86D-08 OVMax= 1.32D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 4.15D-07 CP: 9.99D-01 1.11D+00 7.43D-01 8.40D-01 1.01D+00

CP: 1.23D+00 1.14D+00 7.30D-01

E= -1658.67592412171 Delta-E= -0.000000017004 Rises=F Damp=F

DIIS: error= 2.41D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67592412171 IErMin= 9 ErrMin= 2.41D-06

ErrMax= 2.41D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.26D-08 BMatP= 5.41D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.498D-04 0.131D-02-0.738D-03-0.454D-02-0.265D-01-0.629D-01

Coeff-Com: 0.448D-01 0.372D+00 0.677D+00

Coeff: -0.498D-04 0.131D-02-0.738D-03-0.454D-02-0.265D-01-0.629D-01

Coeff: 0.448D-01 0.372D+00 0.677D+00

Gap= 0.119 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.52D-07 MaxDP=1.44D-05 DE=-1.70D-08 OVMax= 5.05D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.33D-07 CP: 9.99D-01 1.11D+00 7.44D-01 8.42D-01 1.02D+00

CP: 1.26D+00 1.21D+00 9.47D-01 8.77D-01

E= -1658.67592412612 Delta-E= -0.000000004412 Rises=F Damp=F

DIIS: error= 8.95D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67592412612 IErMin=10 ErrMin= 8.95D-07

ErrMax= 8.95D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.88D-09 BMatP= 1.26D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.623D-04 0.119D-02 0.631D-03-0.445D-03-0.125D-01-0.421D-01

Coeff-Com: -0.288D-01 0.112D+00 0.373D+00 0.597D+00

Coeff: -0.623D-04 0.119D-02 0.631D-03-0.445D-03-0.125D-01-0.421D-01

Coeff: -0.288D-01 0.112D+00 0.373D+00 0.597D+00

Gap= 0.119 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.23D-07 MaxDP=5.16D-06 DE=-4.41D-09 OVMax= 1.57D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 5.86D-08 CP: 9.99D-01 1.11D+00 7.44D-01 8.43D-01 1.02D+00

CP: 1.27D+00 1.24D+00 9.65D-01 9.88D-01 8.84D-01

E= -1658.67592412667 Delta-E= -0.000000000542 Rises=F Damp=F

DIIS: error= 3.01D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67592412667 IErMin=11 ErrMin= 3.01D-07

ErrMax= 3.01D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.40D-10 BMatP= 1.88D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.117D-04 0.134D-03 0.319D-03 0.643D-03 0.843D-03-0.184D-02

Coeff-Com: -0.167D-01-0.297D-01-0.713D-03 0.183D+00 0.864D+00

Coeff: -0.117D-04 0.134D-03 0.319D-03 0.643D-03 0.843D-03-0.184D-02

Coeff: -0.167D-01-0.297D-01-0.713D-03 0.183D+00 0.864D+00

Gap= 0.119 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.85D-08 MaxDP=2.06D-06 DE=-5.42D-10 OVMax= 5.86D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 2.54D-08 CP: 9.99D-01 1.11D+00 7.44D-01 8.43D-01 1.02D+00

CP: 1.27D+00 1.25D+00 9.75D-01 1.05D+00 1.02D+00

CP: 1.19D+00

E= -1658.67592412676 Delta-E= -0.000000000096 Rises=F Damp=F

DIIS: error= 2.13D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.67592412676 IErMin=12 ErrMin= 2.13D-07

ErrMax= 2.13D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.10D-11 BMatP= 1.40D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.413D-05-0.128D-03 0.664D-04 0.411D-03 0.248D-02 0.586D-02

Coeff-Com: -0.406D-02-0.339D-01-0.613D-01 0.111D-02 0.458D+00 0.631D+00

Coeff: 0.413D-05-0.128D-03 0.664D-04 0.411D-03 0.248D-02 0.586D-02

Coeff: -0.406D-02-0.339D-01-0.613D-01 0.111D-02 0.458D+00 0.631D+00

Gap= 0.119 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.92D-08 MaxDP=8.92D-07 DE=-9.64D-11 OVMax= 1.68D-06

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.12D-08 CP: 9.99D-01 1.11D+00 7.44D-01 8.43D-01 1.02D+00

CP: 1.27D+00 1.25D+00 9.76D-01 1.06D+00 1.09D+00

CP: 1.33D+00 8.23D-01

E= -1658.67592412678 Delta-E= -0.000000000020 Rises=F Damp=F

DIIS: error= 6.78D-08 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1658.67592412678 IErMin=13 ErrMin= 6.78D-08

ErrMax= 6.78D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.62D-12 BMatP= 5.10D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.351D-05-0.691D-04-0.248D-04 0.581D-04 0.812D-03 0.246D-02

Coeff-Com: 0.176D-02-0.706D-02-0.226D-01-0.342D-01 0.238D-02 0.237D+00

Coeff-Com: 0.820D+00

Coeff: 0.351D-05-0.691D-04-0.248D-04 0.581D-04 0.812D-03 0.246D-02

Coeff: 0.176D-02-0.706D-02-0.226D-01-0.342D-01 0.238D-02 0.237D+00

Coeff: 0.820D+00

Gap= 0.119 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=9.57D-09 MaxDP=5.40D-07 DE=-2.05D-11 OVMax= 1.06D-06

Error on total polarization charges = 0.04175

SCF Done: E(UB3LYP) = -1658.67592413 A.U. after 13 cycles

NFock= 13 Conv=0.96D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655170722582D+03 PE=-6.143221768426D+03 EE= 1.729119679486D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.60

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:53:40 2019, MaxMem= 1342177280 cpu: 326.6

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 342

Leave Link 701 at Sat Aug 17 17:53:41 2019, MaxMem= 1342177280 cpu: 10.3

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:53:41 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:53:44 2019, MaxMem= 1342177280 cpu: 38.4

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.45571923D+00-3.14723558D+00 6.31012811D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000786359 0.004965229 -0.006522408

2 6 -0.004534203 -0.007388031 -0.003603333

3 8 0.001650964 -0.004455345 0.003801607

4 8 0.002347422 0.001009745 0.004964832

5 6 -0.001968044 0.002313448 0.001946914

6 16 -0.000245872 0.002615888 0.003430231

7 6 -0.000792065 0.002963247 0.000573939

8 16 -0.000622953 -0.001684689 0.001957310

9 16 -0.001393447 -0.002590274 -0.001061453

10 6 0.000081451 -0.001765237 -0.003291925

11 6 -0.000704573 -0.000309066 -0.000098504

12 6 0.000009405 0.000167230 -0.000005942

13 6 0.001023470 -0.002072752 0.000571658

14 1 0.001729749 0.003192649 -0.003170551

15 1 0.000574927 0.002363237 -0.000955887

16 1 0.001973039 -0.001392969 0.001431768

17 1 0.000860986 -0.001037360 -0.000186963

18 1 0.000482616 -0.001067978 -0.000611247

19 1 0.001356376 0.001122513 0.001562824

20 1 -0.000344243 -0.000245589 0.000159176

21 1 -0.000113665 0.001668011 -0.000394253

22 1 0.001290460 -0.000001101 0.000253909

23 1 0.000054188 -0.000330883 0.000721893

24 1 -0.000726873 -0.000058678 -0.000488089

25 1 -0.000894409 0.000055012 -0.000302493

26 1 -0.000307308 0.001128837 -0.000615350

27 1 -0.000001040 0.000834904 -0.000067662

-------------------------------------------------------------------

Cartesian Forces: Max 0.007388031 RMS 0.002106394

Leave Link 716 at Sat Aug 17 17:53:44 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.005362970 RMS 0.001502811

Search for a local minimum.

Step number 51 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .15028D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43 45 44 47 46

49 48 51 50

ITU= 0 0 0 0 0 0 0 1 1 1 1 1 -1 -1 0 -1 -1 -1 0 -1

ITU= 0 0 -1 -1 0 0 -1 0 0 -1 1 -1 1 -1 1 1 -1 1 -1 1

ITU= 1 -1 0 0 -1 0 0 -1 -1 0 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.99330.

Iteration 1 RMS(Cart)= 0.08501381 RMS(Int)= 0.00256524

Iteration 2 RMS(Cart)= 0.00383404 RMS(Int)= 0.00000744

Iteration 3 RMS(Cart)= 0.00001261 RMS(Int)= 0.00000059

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000059

ITry= 1 IFail=0 DXMaxC= 2.94D-01 DCOld= 1.00D+10 DXMaxT= 1.20D-01 DXLimC= 3.00D+00 Rises=T

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.85164 -0.00499 -0.01592 0.00000 -0.01592 2.83572

R2 2.29673 -0.00536 -0.00742 0.00000 -0.00742 2.28931

R3 2.55672 -0.00391 -0.00356 0.00000 -0.00356 2.55316

R4 2.85872 0.00303 0.00636 0.00000 0.00636 2.86508

R5 3.63775 -0.00345 -0.02709 0.00000 -0.02709 3.61066

R6 2.05459 0.00120 0.00348 0.00000 0.00348 2.05807

R7 1.83682 -0.00058 0.00011 0.00000 0.00011 1.83693

R8 2.05785 0.00156 0.00339 0.00000 0.00339 2.06124

R9 2.07127 -0.00058 -0.00264 0.00000 -0.00264 2.06862

R10 2.05555 0.00130 0.00450 0.00000 0.00450 2.06005

R11 3.31640 -0.00235 -0.00124 0.00000 -0.00124 3.31516

R12 3.38272 0.00122 0.00494 0.00000 0.00494 3.38765

R13 3.26631 -0.00292 -0.01245 0.00000 -0.01245 3.25386

R14 3.46916 0.00063 0.00313 0.00000 0.00313 3.47229

R15 2.88638 -0.00094 -0.00501 0.00000 -0.00501 2.88137

R16 2.06589 -0.00056 -0.00163 0.00000 -0.00163 2.06426

R17 2.05873 -0.00002 0.00134 0.00000 0.00134 2.06008

R18 2.89529 -0.00091 -0.00116 0.00000 -0.00116 2.89413

R19 2.07582 -0.00134 -0.00362 0.00000 -0.00362 2.07220

R20 2.07249 -0.00032 -0.00136 0.00000 -0.00136 2.07114

R21 2.88560 -0.00007 0.00062 0.00000 0.00062 2.88622

R22 2.07393 -0.00077 -0.00202 0.00000 -0.00202 2.07191

R23 2.07327 -0.00050 -0.00147 0.00000 -0.00147 2.07180

R24 2.06977 -0.00078 -0.00213 0.00000 -0.00213 2.06764

R25 2.07320 -0.00116 -0.00397 0.00000 -0.00397 2.06923

R26 2.07074 -0.00043 -0.00168 0.00000 -0.00168 2.06906

A1 2.15721 0.00438 0.01906 0.00000 0.01906 2.17627

A2 1.99464 -0.00524 -0.01714 0.00000 -0.01714 1.97750

A3 2.12866 0.00099 0.00018 0.00000 0.00018 2.12884

A4 2.03192 -0.00217 -0.00445 0.00000 -0.00445 2.02748

A5 1.81631 0.00124 0.01272 0.00000 0.01272 1.82903

A6 1.86367 0.00055 0.01012 0.00000 0.01012 1.87380

A7 1.93843 0.00118 0.00827 0.00000 0.00827 1.94670

A8 1.92129 0.00203 0.01993 0.00000 0.01993 1.94122

A9 1.88422 -0.00310 -0.05212 0.00000 -0.05212 1.83210

A10 1.89455 -0.00418 -0.02222 0.00000 -0.02222 1.87233

A11 1.89115 0.00320 0.02178 0.00000 0.02178 1.91293

A12 1.91560 0.00134 0.01077 0.00000 0.01077 1.92637

A13 1.96649 -0.00121 -0.01411 0.00000 -0.01411 1.95238

A14 1.88158 -0.00134 0.00188 0.00000 0.00188 1.88346

A15 1.90577 -0.00142 -0.01149 0.00000 -0.01149 1.89428

A16 1.90138 -0.00060 -0.00856 0.00000 -0.00856 1.89281

A17 1.81192 -0.00148 -0.01312 0.00000 -0.01312 1.79880

A18 1.96636 -0.00092 0.00379 0.00000 0.00379 1.97015

A19 2.15324 -0.00098 -0.01032 0.00000 -0.01032 2.14293

A20 2.15299 0.00187 0.00214 0.00000 0.00214 2.15513

A21 1.81128 -0.00123 -0.01573 0.00000 -0.01573 1.79555

A22 1.91062 0.00177 0.01589 0.00000 0.01589 1.92651

A23 1.86097 0.00096 0.01816 0.00000 0.01816 1.87913

A24 1.90754 -0.00142 -0.01544 0.00000 -0.01544 1.89210

A25 1.93263 -0.00057 0.00665 0.00000 0.00666 1.93928

A26 1.95185 -0.00039 -0.01372 0.00000 -0.01372 1.93813

A27 1.89786 -0.00030 -0.01106 0.00000 -0.01106 1.88681

A28 1.95892 -0.00078 -0.00594 0.00000 -0.00594 1.95299

A29 1.92392 -0.00039 -0.00788 0.00000 -0.00788 1.91604

A30 1.90202 0.00129 0.01507 0.00000 0.01507 1.91708

A31 1.91165 0.00038 -0.00470 0.00000 -0.00470 1.90695

A32 1.91076 -0.00059 -0.00231 0.00000 -0.00231 1.90845

A33 1.85352 0.00015 0.00644 0.00000 0.00644 1.85996

A34 1.96468 0.00009 0.00137 0.00000 0.00137 1.96605

A35 1.90481 0.00018 0.00133 0.00000 0.00133 1.90614

A36 1.91303 -0.00056 -0.00516 0.00000 -0.00516 1.90787

A37 1.91431 -0.00026 -0.00149 0.00000 -0.00149 1.91282

A38 1.90689 0.00062 0.00595 0.00000 0.00595 1.91283

A39 1.85701 -0.00008 -0.00222 0.00000 -0.00222 1.85479

A40 1.95078 -0.00050 -0.00526 0.00000 -0.00526 1.94552

A41 1.94409 -0.00051 -0.00198 0.00000 -0.00198 1.94211

A42 1.94676 -0.00038 -0.00393 0.00000 -0.00393 1.94283

A43 1.87293 0.00055 0.00400 0.00000 0.00400 1.87693

A44 1.87795 0.00021 -0.00083 0.00000 -0.00083 1.87712

A45 1.86711 0.00073 0.00883 0.00000 0.00883 1.87594

D1 2.69386 -0.00067 0.02382 0.00000 0.02382 2.71768

D2 -1.45021 0.00043 0.04125 0.00000 0.04125 -1.40895

D3 0.54036 -0.00228 -0.00754 0.00000 -0.00754 0.53282

D4 -0.52500 0.00120 0.06513 0.00000 0.06513 -0.45988

D5 1.61412 0.00230 0.08256 0.00000 0.08256 1.69668

D6 -2.67850 -0.00040 0.03377 0.00000 0.03377 -2.64473

D7 -3.13218 0.00003 0.03185 0.00000 0.03185 -3.10033

D8 -0.06644 0.00204 0.07285 0.00000 0.07285 0.00641

D9 3.12727 -0.00034 0.01177 0.00000 0.01178 3.13905

D10 -1.10543 0.00065 0.03338 0.00000 0.03338 -1.07205

D11 1.01667 0.00002 0.02048 0.00000 0.02048 1.03716

D12 1.05332 -0.00136 -0.00844 0.00000 -0.00844 1.04489

D13 3.10381 -0.00037 0.01317 0.00000 0.01317 3.11697

D14 -1.05728 -0.00100 0.00027 0.00000 0.00027 -1.05701

D15 -1.03253 0.00044 0.03850 0.00000 0.03850 -0.99403

D16 1.01795 0.00143 0.06011 0.00000 0.06011 1.07806

D17 3.14005 0.00080 0.04721 0.00000 0.04721 -3.09592

D18 -3.10603 0.00106 0.01843 0.00000 0.01843 -3.08760

D19 -0.90657 -0.00008 0.02651 0.00000 0.02651 -0.88006

D20 1.20129 0.00115 0.02277 0.00000 0.02277 1.22406

D21 1.78031 0.00094 0.04240 0.00000 0.04240 1.82271

D22 -1.20987 0.00100 0.07041 0.00000 0.07041 -1.13947

D23 2.67704 -0.00060 -0.08439 0.00000 -0.08439 2.59265

D24 -0.61594 -0.00094 -0.11387 0.00000 -0.11387 -0.72981

D25 -3.06616 0.00005 0.03548 0.00000 0.03548 -3.03068

D26 -0.97476 0.00089 0.06360 0.00000 0.06360 -0.91116

D27 1.07377 0.00033 0.05236 0.00000 0.05236 1.12613

D28 3.11748 0.00090 0.04129 0.00000 0.04129 -3.12441

D29 -1.02968 0.00057 0.02569 0.00000 0.02569 -1.00399

D30 0.99801 0.00127 0.03773 0.00000 0.03773 1.03573

D31 1.07061 -0.00101 0.00473 0.00000 0.00473 1.07533

D32 -3.07656 -0.00134 -0.01088 0.00000 -0.01088 -3.08743

D33 -1.04887 -0.00064 0.00116 0.00000 0.00116 -1.04771

D34 -1.04902 0.00006 0.02356 0.00000 0.02356 -1.02546

D35 1.08700 -0.00027 0.00796 0.00000 0.00796 1.09496

D36 3.11469 0.00043 0.01999 0.00000 0.01999 3.13468

D37 3.13271 -0.00022 0.01801 0.00000 0.01801 -3.13247

D38 -1.02075 -0.00036 0.01796 0.00000 0.01796 -1.00278

D39 1.00661 -0.00067 0.01316 0.00000 0.01316 1.01977

D40 0.98974 0.00054 0.03532 0.00000 0.03532 1.02506

D41 3.11947 0.00040 0.03528 0.00000 0.03528 -3.12844

D42 -1.13635 0.00010 0.03047 0.00000 0.03047 -1.10588

D43 -1.03602 0.00049 0.03155 0.00000 0.03155 -1.00447

D44 1.09371 0.00035 0.03151 0.00000 0.03151 1.12522

D45 3.12107 0.00004 0.02670 0.00000 0.02670 -3.13542

D46 3.13125 0.00000 0.00538 0.00000 0.00538 3.13663

D47 -1.05692 0.00001 0.00554 0.00000 0.00554 -1.05138

D48 1.02797 0.00034 0.01276 0.00000 0.01276 1.04073

D49 1.00690 -0.00011 0.00382 0.00000 0.00382 1.01072

D50 3.10192 -0.00010 0.00398 0.00000 0.00398 3.10590

D51 -1.09638 0.00023 0.01119 0.00000 0.01119 -1.08518

D52 -1.02236 -0.00022 0.00395 0.00000 0.00395 -1.01841

D53 1.07266 -0.00021 0.00411 0.00000 0.00411 1.07676

D54 -3.12564 0.00012 0.01132 0.00000 0.01132 -3.11432

Item Value Threshold Converged?

Maximum Force 0.005363 0.000450 NO

RMS Force 0.001503 0.000300 NO

Maximum Displacement 0.293888 0.001800 NO

RMS Displacement 0.084289 0.001200 NO

Predicted change in Energy=-4.515419D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:53:44 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.094822 -0.406975 -0.206048

2 6 0 -2.844980 0.074083 0.470906

3 8 0 -4.887930 0.308002 -0.778237

4 8 0 -4.244892 -1.748905 -0.160115

5 6 0 -2.299969 -0.810348 1.575176

6 16 0 -1.577871 0.292807 -0.942351

7 6 0 -0.116252 0.765097 -0.094885

8 16 0 1.082929 -0.562499 0.019648

9 16 0 0.021960 2.247205 0.770609

10 6 0 2.687712 0.332154 -0.002811

11 6 0 3.846181 -0.656937 -0.070051

12 6 0 5.203624 0.052179 -0.066095

13 6 0 6.376626 -0.922718 -0.145870

14 1 0 -3.039226 1.082599 0.833211

15 1 0 -5.054499 -1.965872 -0.652423

16 1 0 -1.394902 -0.363595 1.988730

17 1 0 -3.030477 -0.902378 2.385230

18 1 0 -2.058714 -1.809840 1.212964

19 1 0 2.685510 0.995155 -0.870954

20 1 0 2.750792 0.948595 0.894094

21 1 0 3.795628 -1.346117 0.781372

22 1 0 3.759605 -1.270317 -0.974197

23 1 0 5.248161 0.750907 -0.909840

24 1 0 5.292232 0.660608 0.841616

25 1 0 7.335701 -0.396089 -0.146793

26 1 0 6.379255 -1.611640 0.705234

27 1 0 6.330776 -1.526797 -1.057899

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.500596 0.000000

3 O 1.211451 2.405976 0.000000

4 O 1.351076 2.383533 2.241972 0.000000

5 C 2.560657 1.516135 3.672438 2.770352 0.000000

6 S 2.714199 1.910680 3.314160 3.448693 2.841886

7 C 4.149112 2.871163 4.841985 4.834267 3.168556

8 S 5.185000 4.004664 6.086505 5.461278 3.731634

9 S 4.994639 3.609934 5.501495 5.919558 3.922666

10 C 6.825715 5.558929 7.615262 7.239928 5.354653

11 C 7.946099 6.752677 8.815743 8.164923 6.364390

12 C 9.310827 8.066528 10.119884 9.619107 7.729271

13 C 10.484313 9.295807 11.349219 10.653611 8.846350

14 H 2.100756 1.089083 2.571862 3.233844 2.163391

15 H 1.884248 3.210180 2.283435 0.972062 3.726241

16 H 3.479727 2.144313 4.506483 3.828716 1.090762

17 H 2.844815 2.156970 3.862987 2.944519 1.094668

18 H 2.850852 2.172102 4.056427 2.582331 1.090131

19 H 6.955643 5.765005 7.605115 7.487699 5.839383

20 H 7.064723 5.679483 7.845835 7.571491 5.391469

21 H 8.007258 6.797870 8.976228 8.105468 6.170371

22 H 7.938982 6.893205 8.792574 8.060010 6.590092

23 H 9.440728 8.237929 10.146617 9.845264 8.098586

24 H 9.505478 8.166740 10.314260 9.887667 7.768097

25 H 11.430682 10.210234 12.260164 11.659350 9.797087

26 H 10.582435 9.379930 11.525414 10.660215 8.759440

27 H 10.520111 9.438991 11.371195 10.616031 9.051858

6 7 8 9 10

6 S 0.000000

7 C 1.754305 0.000000

8 S 2.955816 1.792669 0.000000

9 S 3.051780 1.721868 3.095809 0.000000

10 C 4.368007 2.838684 1.837454 3.372215 0.000000

11 C 5.575236 4.209948 2.766320 4.874979 1.524753

12 C 6.842105 5.367510 4.167171 5.689276 2.532233

13 C 8.086155 6.708858 5.308519 7.160316 3.899135

14 H 2.431450 3.083172 4.512249 3.275833 5.836087

15 H 4.156035 5.670566 6.331600 6.748738 8.102145

16 H 3.009249 2.692647 3.171198 3.210544 4.595437

17 H 3.822476 4.174225 4.757268 4.673782 6.318583

18 H 3.049216 3.480507 3.584660 4.580884 5.347412

19 H 4.321436 2.916347 2.405769 3.369994 1.092359

20 H 4.747622 3.038370 2.414504 3.024593 1.090145

21 H 5.876376 4.530768 2.924555 5.210821 2.158476

22 H 5.561747 4.465240 2.941654 5.421006 2.158810

23 H 6.841464 5.425982 4.465215 5.689991 2.748446

24 H 7.107470 5.489959 4.459805 5.504371 2.757619

25 H 8.975481 7.542059 6.257201 7.830673 4.706896

26 H 8.346096 6.962807 5.442591 7.437080 4.231685

27 H 8.116096 6.909728 5.443425 7.575467 4.223840

11 12 13 14 15

11 C 0.000000

12 C 1.531507 0.000000

13 C 2.545494 1.527324 0.000000

14 H 7.158959 8.355543 9.676681 0.000000

15 H 9.015241 10.471170 11.489794 3.944821 0.000000

16 H 5.638580 6.923563 8.078724 2.475985 4.789116

17 H 7.305961 8.644108 9.741687 2.519717 3.801976

18 H 6.151675 7.605569 8.590016 3.077632 3.532526

19 H 2.172098 2.806760 4.222359 5.973644 8.289944

20 H 2.169604 2.782429 4.210701 5.791889 8.473984

21 H 1.096561 2.157750 2.774994 7.253729 8.986914

22 H 1.095998 2.158433 2.766902 7.418021 8.847360

23 H 2.157040 1.096408 2.158264 8.475201 10.657953

24 H 2.158269 1.096348 2.158231 8.342142 10.778933

25 H 3.500098 2.180185 1.094150 10.525495 12.499478

26 H 2.815846 2.178383 1.094988 9.797096 11.519525

27 H 2.811710 2.178832 1.094902 9.908692 11.400951

16 17 18 19 20

16 H 0.000000

17 H 1.767089 0.000000

18 H 1.770335 1.772573 0.000000

19 H 5.164665 6.846596 5.892230 0.000000

20 H 4.484067 6.250813 5.553557 1.766869 0.000000

21 H 5.418918 7.026022 5.888518 3.073125 2.523904

22 H 6.014153 7.584612 6.239199 2.509323 3.071121

23 H 7.333084 9.062378 8.028335 2.574558 3.087087

24 H 6.861678 8.607738 7.763854 3.136848 2.558242

25 H 8.988045 10.682936 9.597014 4.907570 4.890093

26 H 7.977625 9.584806 8.455555 4.787849 4.444796

27 H 8.385767 9.993903 8.696004 4.436570 4.770129

21 22 23 24 25

21 H 0.000000

22 H 1.757574 0.000000

23 H 3.060647 2.511033 0.000000

24 H 2.504077 3.061796 1.754337 0.000000

25 H 3.781026 3.773239 2.501133 2.503863 0.000000

26 H 2.598351 3.130424 3.077250 2.522565 1.765871

27 H 3.137281 2.585287 2.526245 3.077576 1.765925

26 27

26 H 0.000000

27 H 1.765838 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 8.08D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.104034 -0.463754 -0.130502

2 6 0 -2.848729 0.119438 0.449055

3 8 0 -4.901241 0.149313 -0.805944

4 8 0 -4.254372 -1.779809 0.135591

5 6 0 -2.295545 -0.573284 1.679011

6 16 0 -1.592569 0.101710 -0.990545

7 6 0 -0.124169 0.703790 -0.242958

8 16 0 1.075245 -0.589242 0.078193

9 16 0 0.021478 2.307322 0.367206

10 6 0 2.680224 0.286881 -0.102607

11 6 0 3.837669 -0.701890 -0.015867

12 6 0 5.195435 -0.004049 -0.138359

13 6 0 6.367321 -0.980895 -0.066419

14 1 0 -3.039673 1.173988 0.642875

15 1 0 -5.067892 -2.073016 -0.308391

16 1 0 -1.387073 -0.066444 2.006966

17 1 0 -3.019762 -0.530225 2.498739

18 1 0 -2.057589 -1.618998 1.483448

19 1 0 2.671568 0.798860 -1.067516

20 1 0 2.750580 1.041691 0.680802

21 1 0 3.793430 -1.242341 0.937234

22 1 0 3.743763 -1.454825 -0.806741

23 1 0 5.233723 0.547088 -1.085403

24 1 0 5.291398 0.744581 0.656827

25 1 0 7.326608 -0.463186 -0.160823

26 1 0 6.376260 -1.521235 0.885921

27 1 0 6.314083 -1.726015 -0.866901

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3047179 0.1933933 0.1808818

Leave Link 202 at Sat Aug 17 17:53:45 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.3238488498 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0549991944 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.2688496554 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2318

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.30D-08

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 94

GePol: Fraction of low-weight points (<1% of avg) = 4.06%

GePol: Cavity surface area = 309.195 Ang\*\*2

GePol: Cavity volume = 320.394 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057848227 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.2630648327 Hartrees.

Leave Link 301 at Sat Aug 17 17:53:45 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:53:45 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:53:45 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Lowest energy guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000168 -0.000011 0.000006 Ang= -0.02 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999747 0.022421 0.001586 -0.000763 Ang= 2.58 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 6.70D-03

Max alpha theta= 4.401 degrees.

Max beta theta= 4.454 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 17:53:45 2019, MaxMem= 1342177280 cpu: 4.5

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16119372.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.22D-15 for 2315.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.77D-15 for 805 86.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.99D-15 for 2315.

Iteration 1 A^-1\*A deviation from orthogonality is 3.95D-10 for 912 739.

Iteration 2 A\*A^-1 deviation from unit magnitude is 3.22D-15 for 195.

Iteration 2 A\*A^-1 deviation from orthogonality is 2.72D-15 for 581 302.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 72.

Iteration 2 A^-1\*A deviation from orthogonality is 4.91D-16 for 728 83.

E= -1658.67701778428

DIIS: error= 7.67D-06 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67701778428 IErMin= 1 ErrMin= 7.67D-06

ErrMax= 7.67D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.69D-08 BMatP= 2.69D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 88.631 Goal= None Shift= 0.000

Gap= 88.630 Goal= None Shift= 0.000

RMSDP=3.46D-07 MaxDP=2.09D-05 OVMax= 3.17D-05

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.46D-07 CP: 1.00D+00

E= -1658.67701778384 Delta-E= 0.000000000442 Rises=F Damp=F

DIIS: error= 7.65D-06 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 1 EnMin= -1658.67701778428 IErMin= 2 ErrMin= 7.65D-06

ErrMax= 7.65D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.77D-08 BMatP= 2.69D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.549D+00 0.451D+00

Coeff: 0.549D+00 0.451D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.26D-07 MaxDP=1.61D-05 DE= 4.42D-10 OVMax= 1.98D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.49D-07 CP: 1.00D+00 5.10D-01

E= -1658.67701779031 Delta-E= -0.000000006469 Rises=F Damp=F

DIIS: error= 1.28D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67701779031 IErMin= 3 ErrMin= 1.28D-06

ErrMax= 1.28D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.63D-09 BMatP= 2.69D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.264D-01 0.172D+00 0.801D+00

Coeff: 0.264D-01 0.172D+00 0.801D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.64D-08 MaxDP=2.99D-06 DE=-6.47D-09 OVMax= 4.19D-06

Cycle 4 Pass 1 IDiag 1:

RMSU= 4.29D-08 CP: 1.00D+00 5.95D-01 8.57D-01

E= -1658.67701779055 Delta-E= -0.000000000242 Rises=F Damp=F

DIIS: error= 4.04D-07 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67701779055 IErMin= 4 ErrMin= 4.04D-07

ErrMax= 4.04D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.28D-10 BMatP= 1.63D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.808D-02 0.763D-01 0.434D+00 0.497D+00

Coeff: -0.808D-02 0.763D-01 0.434D+00 0.497D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.68D-08 MaxDP=1.20D-06 DE=-2.42D-10 OVMax= 2.64D-06

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.27D-08 CP: 1.00D+00 5.92D-01 9.11D-01 4.83D-01

E= -1658.67701779062 Delta-E= -0.000000000064 Rises=F Damp=F

DIIS: error= 1.34D-07 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67701779062 IErMin= 5 ErrMin= 1.34D-07

ErrMax= 1.34D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.28D-11 BMatP= 2.28D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.746D-02 0.329D-01 0.200D+00 0.296D+00 0.478D+00

Coeff: -0.746D-02 0.329D-01 0.200D+00 0.296D+00 0.478D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=8.68D-09 MaxDP=3.75D-07 DE=-6.41D-11 OVMax= 9.12D-07

Error on total polarization charges = 0.04162

SCF Done: E(UB3LYP) = -1658.67701779 A.U. after 5 cycles

NFock= 5 Conv=0.87D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655236136576D+03 PE=-6.147292110389D+03 EE= 1.731115891190D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.63

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:53:59 2019, MaxMem= 1342177280 cpu: 151.2

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 335

Leave Link 701 at Sat Aug 17 17:54:00 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:54:00 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:54:03 2019, MaxMem= 1342177280 cpu: 38.6

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.40717422D+00-2.94596105D+00 6.35969704D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000013763 -0.000010729 0.000033882

2 6 -0.000007887 -0.000077004 0.000002337

3 8 -0.000036341 0.000108438 0.000021882

4 8 0.000068029 -0.000028569 -0.000003303

5 6 -0.000037519 -0.000036294 0.000024032

6 16 0.000052242 0.000066890 0.000004597

7 6 -0.000031306 0.000027755 0.000020053

8 16 0.000010494 0.000011894 0.000006258

9 16 -0.000027423 -0.000047919 0.000060788

10 6 0.000030535 -0.000012003 0.000022801

11 6 -0.000010305 0.000005453 -0.000012196

12 6 -0.000000955 0.000008997 -0.000020958

13 6 0.000004773 0.000001747 -0.000009124

14 1 -0.000011947 0.000017271 0.000018823

15 1 -0.000009529 0.000042311 -0.000044207

16 1 0.000018119 -0.000036000 0.000004952

17 1 0.000008195 -0.000052880 -0.000008072

18 1 0.000009110 -0.000028690 -0.000047619

19 1 0.000025975 0.000031537 0.000021261

20 1 -0.000039200 -0.000027264 0.000036633

21 1 0.000000059 -0.000012514 -0.000032781

22 1 0.000001333 0.000007957 -0.000034733

23 1 0.000006085 0.000035769 0.000013543

24 1 -0.000000593 -0.000019025 0.000020025

25 1 0.000001143 0.000010948 -0.000011706

26 1 -0.000003876 -0.000024781 -0.000042990

27 1 -0.000005447 0.000036705 -0.000044178

-------------------------------------------------------------------

Cartesian Forces: Max 0.000108438 RMS 0.000030961

Leave Link 716 at Sat Aug 17 17:54:03 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000105557 RMS 0.000021903

Search for a local minimum.

Step number 52 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .21903D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43 45 44 47 46

49 48 51 50 52

ITU= 0 0 0 0 0 0 0 0 1 1 1 1 1 -1 -1 0 -1 -1 -1 0

ITU= -1 0 0 -1 -1 0 0 -1 0 0 -1 1 -1 1 -1 1 1 -1 1 -1

ITU= 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Use linear search instead of GDIIS.

Eigenvalues --- -0.00111 0.00000 0.00000 0.00074 0.00206

Eigenvalues --- 0.00241 0.00281 0.00375 0.01112 0.01856

Eigenvalues --- 0.01978 0.03197 0.03461 0.03721 0.04136

Eigenvalues --- 0.04595 0.04808 0.04848 0.05202 0.05240

Eigenvalues --- 0.05457 0.05505 0.05607 0.05909 0.06512

Eigenvalues --- 0.08174 0.08332 0.09830 0.10701 0.11399

Eigenvalues --- 0.12107 0.12284 0.14795 0.15389 0.15738

Eigenvalues --- 0.15917 0.15965 0.16201 0.16722 0.17149

Eigenvalues --- 0.18930 0.20140 0.21104 0.21849 0.22393

Eigenvalues --- 0.22863 0.23087 0.23994 0.25037 0.26499

Eigenvalues --- 0.26968 0.28446 0.29316 0.29482 0.29734

Eigenvalues --- 0.30127 0.30984 0.32797 0.33693 0.33866

Eigenvalues --- 0.33881 0.33928 0.33984 0.34027 0.34037

Eigenvalues --- 0.34109 0.34214 0.34379 0.34576 0.34885

Eigenvalues --- 0.35149 0.36856 0.48667 0.52599 0.85442

Eigenvalue 1 is -1.11D-03 should be greater than 0.000000 Eigenvector:

D23 D24 D1 D3 D4

1 0.43045 0.32924 -0.29057 -0.26936 -0.25756

D2 D6 D20 D5 D18

1 -0.23951 -0.23635 -0.21339 -0.20650 -0.20186

RFO step: Lambda=-1.11438845D-03 EMin=-1.11219202D-03

I= 1 Eig= -1.11D-03 Dot1= 1.48D-05

I= 1 Stepn= 2.99D-01 RXN= 2.99D-01 EDone=F

Mixed 1 eigenvectors in step. Raw Step.Grad= 1.48D-05.

RFO eigenvector is Hessian eigenvector with negative curvature.

Taking step of 2.99D-01 in eigenvector direction(s). Step.Grad= -1.40D-05.

Quartic linear search produced a step of -0.00140.

Iteration 1 RMS(Cart)= 0.09047813 RMS(Int)= 0.00277915

Iteration 2 RMS(Cart)= 0.00497407 RMS(Int)= 0.00003098

Iteration 3 RMS(Cart)= 0.00000668 RMS(Int)= 0.00003072

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00003072

ITry= 1 IFail=0 DXMaxC= 3.20D-01 DCOld= 1.00D+10 DXMaxT= 1.20D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83572 -0.00004 0.00000 -0.01085 -0.01086 2.82486

R2 2.28931 0.00007 0.00000 0.00793 0.00793 2.29724

R3 2.55316 0.00002 0.00000 -0.00417 -0.00417 2.54900

R4 2.86508 0.00001 0.00000 0.00658 0.00658 2.87166

R5 3.61066 0.00004 0.00000 -0.00420 -0.00420 3.60646

R6 2.05807 0.00002 0.00000 0.00025 0.00025 2.05832

R7 1.83693 0.00001 0.00000 -0.00058 -0.00058 1.83636

R8 2.06124 0.00002 0.00000 0.00051 0.00051 2.06175

R9 2.06862 0.00000 0.00000 -0.00015 -0.00015 2.06847

R10 2.06005 0.00001 0.00000 -0.00258 -0.00258 2.05747

R11 3.31516 -0.00005 0.00000 0.00521 0.00521 3.32036

R12 3.38765 0.00003 0.00000 0.00193 0.00193 3.38959

R13 3.25386 -0.00003 0.00000 -0.00250 -0.00250 3.25136

R14 3.47229 0.00000 0.00000 -0.00212 -0.00212 3.47016

R15 2.88137 0.00000 0.00000 0.00203 0.00203 2.88339

R16 2.06426 0.00001 0.00000 -0.00068 -0.00068 2.06358

R17 2.06008 0.00000 0.00000 -0.00233 -0.00233 2.05775

R18 2.89413 0.00001 0.00000 -0.00121 -0.00121 2.89292

R19 2.07220 0.00000 0.00000 -0.00142 -0.00142 2.07078

R20 2.07114 0.00002 0.00000 0.00020 0.00020 2.07133

R21 2.88622 0.00000 0.00000 -0.00019 -0.00019 2.88603

R22 2.07191 0.00001 0.00000 -0.00056 -0.00056 2.07135

R23 2.07180 0.00000 0.00000 -0.00066 -0.00066 2.07114

R24 2.06764 0.00000 0.00000 -0.00057 -0.00057 2.06708

R25 2.06923 0.00001 0.00000 -0.00053 -0.00053 2.06870

R26 2.06906 0.00000 0.00000 -0.00067 -0.00067 2.06840

A1 2.17627 -0.00002 0.00000 -0.00077 -0.00079 2.17548

A2 1.97750 -0.00005 0.00000 -0.00332 -0.00334 1.97416

A3 2.12884 0.00008 0.00000 0.00441 0.00439 2.13323

A4 2.02748 -0.00001 0.00000 -0.00026 -0.00030 2.02718

A5 1.82903 0.00004 0.00000 0.00367 0.00363 1.83266

A6 1.87380 -0.00001 0.00000 0.00593 0.00594 1.87973

A7 1.94670 -0.00001 0.00000 0.00982 0.00981 1.95651

A8 1.94122 0.00001 0.00000 -0.00828 -0.00826 1.93295

A9 1.83210 -0.00001 0.00000 -0.01152 -0.01150 1.82060

A10 1.87233 -0.00003 0.00000 -0.00905 -0.00905 1.86328

A11 1.91293 -0.00001 0.00000 -0.00609 -0.00609 1.90683

A12 1.92637 0.00001 0.00000 -0.00026 -0.00026 1.92611

A13 1.95238 -0.00001 0.00000 0.00139 0.00139 1.95377

A14 1.88346 0.00000 0.00000 -0.00215 -0.00217 1.88129

A15 1.89428 0.00000 0.00000 0.00511 0.00511 1.89939

A16 1.89281 0.00001 0.00000 0.00204 0.00204 1.89485

A17 1.79880 -0.00011 0.00000 -0.00662 -0.00662 1.79218

A18 1.97015 0.00001 0.00000 -0.02404 -0.02419 1.94596

A19 2.14293 -0.00004 0.00000 0.00067 0.00054 2.14347

A20 2.15513 0.00002 0.00000 0.01836 0.01820 2.17333

A21 1.79555 0.00007 0.00000 0.01082 0.01082 1.80637

A22 1.92651 0.00002 0.00000 -0.00332 -0.00333 1.92318

A23 1.87913 0.00002 0.00000 0.00862 0.00859 1.88772

A24 1.89210 -0.00004 0.00000 -0.00402 -0.00401 1.88809

A25 1.93928 -0.00002 0.00000 -0.01283 -0.01282 1.92646

A26 1.93813 0.00002 0.00000 0.00911 0.00913 1.94726

A27 1.88681 0.00000 0.00000 0.00270 0.00273 1.88953

A28 1.95299 -0.00002 0.00000 -0.00307 -0.00307 1.94992

A29 1.91604 0.00000 0.00000 0.00312 0.00312 1.91916

A30 1.91708 0.00002 0.00000 -0.00216 -0.00215 1.91493

A31 1.90695 0.00001 0.00000 -0.00029 -0.00028 1.90667

A32 1.90845 0.00000 0.00000 0.00465 0.00464 1.91310

A33 1.85996 -0.00001 0.00000 -0.00218 -0.00218 1.85778

A34 1.96605 0.00000 0.00000 0.00187 0.00186 1.96791

A35 1.90614 0.00001 0.00000 0.00396 0.00395 1.91009

A36 1.90787 -0.00001 0.00000 -0.00408 -0.00407 1.90380

A37 1.91282 0.00000 0.00000 0.00043 0.00042 1.91323

A38 1.91283 0.00000 0.00000 -0.00233 -0.00233 1.91051

A39 1.85479 0.00000 0.00000 0.00006 0.00006 1.85485

A40 1.94552 0.00000 0.00000 -0.00064 -0.00064 1.94488

A41 1.94211 0.00000 0.00000 0.00235 0.00235 1.94446

A42 1.94283 -0.00001 0.00000 -0.00014 -0.00014 1.94269

A43 1.87693 0.00000 0.00000 -0.00065 -0.00065 1.87628

A44 1.87712 0.00000 0.00000 -0.00097 -0.00097 1.87615

A45 1.87594 0.00000 0.00000 -0.00006 -0.00006 1.87588

D1 2.71768 -0.00002 0.00000 -0.08694 -0.08693 2.63074

D2 -1.40895 -0.00001 0.00000 -0.07166 -0.07166 -1.48061

D3 0.53282 -0.00001 0.00000 -0.08059 -0.08058 0.45224

D4 -0.45988 -0.00002 0.00000 -0.07706 -0.07706 -0.53694

D5 1.69668 -0.00001 0.00000 -0.06178 -0.06179 1.63489

D6 -2.64473 -0.00002 0.00000 -0.07071 -0.07071 -2.71545

D7 -3.10033 0.00000 0.00000 -0.02379 -0.02380 -3.12412

D8 0.00641 0.00000 0.00000 -0.01433 -0.01431 -0.00790

D9 3.13905 0.00001 0.00000 0.01230 0.01230 -3.13183

D10 -1.07205 0.00001 0.00000 0.00574 0.00575 -1.06630

D11 1.03716 0.00002 0.00000 0.00908 0.00909 1.04625

D12 1.04489 -0.00002 0.00000 -0.00022 -0.00023 1.04465

D13 3.11697 -0.00001 0.00000 -0.00679 -0.00679 3.11018

D14 -1.05701 -0.00001 0.00000 -0.00344 -0.00345 -1.06045

D15 -0.99403 0.00000 0.00000 0.01322 0.01322 -0.98081

D16 1.07806 0.00000 0.00000 0.00665 0.00666 1.08472

D17 -3.09592 0.00000 0.00000 0.01000 0.01000 -3.08592

D18 -3.08760 0.00001 0.00000 -0.06040 -0.06043 3.13516

D19 -0.88006 0.00001 0.00000 -0.05211 -0.05208 -0.93214

D20 1.22406 0.00002 0.00000 -0.06385 -0.06384 1.16021

D21 1.82271 -0.00003 0.00000 0.01943 0.01955 1.84225

D22 -1.13947 0.00003 0.00000 0.04734 0.04722 -1.09224

D23 2.59265 0.00004 0.00000 0.12879 0.12887 2.72152

D24 -0.72981 -0.00002 0.00000 0.09851 0.09842 -0.63139

D25 -3.03068 -0.00001 0.00000 0.00468 0.00470 -3.02599

D26 -0.91116 -0.00001 0.00000 -0.00759 -0.00760 -0.91876

D27 1.12613 -0.00002 0.00000 -0.00192 -0.00192 1.12421

D28 -3.12441 0.00001 0.00000 -0.00589 -0.00587 -3.13028

D29 -1.00399 0.00001 0.00000 -0.00614 -0.00613 -1.01012

D30 1.03573 0.00001 0.00000 -0.00823 -0.00822 1.02752

D31 1.07533 -0.00001 0.00000 -0.00624 -0.00625 1.06908

D32 -3.08743 -0.00001 0.00000 -0.00650 -0.00651 -3.09395

D33 -1.04771 -0.00001 0.00000 -0.00858 -0.00860 -1.05631

D34 -1.02546 -0.00001 0.00000 -0.00716 -0.00716 -1.03262

D35 1.09496 -0.00001 0.00000 -0.00742 -0.00742 1.08754

D36 3.13468 -0.00001 0.00000 -0.00950 -0.00950 3.12518

D37 -3.13247 -0.00001 0.00000 -0.01220 -0.01220 3.13851

D38 -1.00278 -0.00001 0.00000 -0.00760 -0.00759 -1.01037

D39 1.01977 -0.00001 0.00000 -0.00759 -0.00759 1.01218

D40 1.02506 0.00000 0.00000 -0.01392 -0.01392 1.01114

D41 -3.12844 0.00000 0.00000 -0.00931 -0.00931 -3.13774

D42 -1.10588 0.00000 0.00000 -0.00930 -0.00931 -1.11519

D43 -1.00447 0.00000 0.00000 -0.01376 -0.01376 -1.01823

D44 1.12522 0.00000 0.00000 -0.00915 -0.00915 1.11607

D45 -3.13542 0.00000 0.00000 -0.00914 -0.00915 3.13862

D46 3.13663 0.00001 0.00000 0.03798 0.03798 -3.10857

D47 -1.05138 0.00001 0.00000 0.03832 0.03832 -1.01306

D48 1.04073 0.00001 0.00000 0.03974 0.03974 1.08047

D49 1.01072 0.00000 0.00000 0.03136 0.03136 1.04208

D50 3.10590 0.00000 0.00000 0.03170 0.03170 3.13759

D51 -1.08518 0.00000 0.00000 0.03312 0.03312 -1.05207

D52 -1.01841 0.00000 0.00000 0.03238 0.03238 -0.98604

D53 1.07676 0.00000 0.00000 0.03272 0.03272 1.10948

D54 -3.11432 0.00000 0.00000 0.03413 0.03414 -3.08018

Item Value Threshold Converged?

Maximum Force 0.000106 0.000450 YES

RMS Force 0.000022 0.000300 YES

Maximum Displacement 0.320174 0.001800 NO

RMS Displacement 0.090647 0.001200 NO

Predicted change in Energy=-6.397387D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:54:03 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.110016 -0.396928 -0.137153

2 6 0 -2.818515 0.054356 0.465299

3 8 0 -4.944938 0.344615 -0.617590

4 8 0 -4.258152 -1.737614 -0.129036

5 6 0 -2.252961 -0.821611 1.570769

6 16 0 -1.616260 0.216968 -1.007913

7 6 0 -0.132454 0.756954 -0.237201

8 16 0 1.079059 -0.562657 -0.146688

9 16 0 -0.009842 2.252637 0.604334

10 6 0 2.679316 0.331422 -0.037570

11 6 0 3.840384 -0.655328 -0.117523

12 6 0 5.193757 0.052605 -0.013766

13 6 0 6.373418 -0.914588 -0.086884

14 1 0 -2.955609 1.076728 0.815085

15 1 0 -5.112132 -1.927719 -0.551991

16 1 0 -1.321013 -0.385767 1.933896

17 1 0 -2.950325 -0.869419 2.413100

18 1 0 -2.055844 -1.835337 1.225930

19 1 0 2.728152 1.043815 -0.863748

20 1 0 2.692948 0.890794 0.896586

21 1 0 3.757743 -1.396080 0.685756

22 1 0 3.787931 -1.212511 -1.059986

23 1 0 5.278217 0.797259 -0.813655

24 1 0 5.235629 0.609025 0.929558

25 1 0 7.327322 -0.390582 0.022636

26 1 0 6.320222 -1.670203 0.703436

27 1 0 6.396122 -1.442468 -1.045458

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.494852 0.000000

3 O 1.215648 2.403866 0.000000

4 O 1.348870 2.374226 2.246339 0.000000

5 C 2.558517 1.519617 3.660019 2.783737 0.000000

6 S 2.711809 1.908458 3.353914 3.401824 2.851953

7 C 4.142759 2.863926 4.845071 4.822442 3.202682

8 S 5.191730 3.993284 6.110109 5.465039 3.757536

9 S 4.937754 3.569371 5.430360 5.874357 3.926395

10 C 6.829015 5.527730 7.646297 7.240010 5.314471

11 C 7.954622 6.721924 8.856175 8.170542 6.325095

12 C 9.315444 8.026582 10.160857 9.620642 7.663460

13 C 10.496328 9.259341 11.400545 10.663462 8.784695

14 H 2.100255 1.089214 2.558510 3.241682 2.160663

15 H 1.876073 3.197527 2.279421 0.971757 3.728866

16 H 3.473889 2.143127 4.491811 3.835356 1.091030

17 H 2.841112 2.159782 3.825890 2.987746 1.094588

18 H 2.854232 2.175125 4.061726 2.587594 1.088765

19 H 7.025968 5.788861 7.708812 7.555434 5.849630

20 H 7.000512 5.591231 7.805661 7.501881 5.277203

21 H 7.973526 6.737917 8.970249 8.064434 6.102607

22 H 7.993395 6.897578 8.881630 8.116764 6.600458

23 H 9.488027 8.230717 10.235049 9.891239 8.063799

24 H 9.459962 8.086558 10.300850 9.836625 7.650937

25 H 11.438456 10.165231 12.310921 11.664506 9.714130

26 H 10.541238 9.303082 11.519914 10.611293 8.658628

27 H 10.597034 9.456871 11.488968 10.697687 9.057414

6 7 8 9 10

6 S 0.000000

7 C 1.757060 0.000000

8 S 2.935007 1.793692 0.000000

9 S 3.053500 1.720547 3.110566 0.000000

10 C 4.405297 2.850787 1.836330 3.366702 0.000000

11 C 5.597201 4.218093 2.763033 4.878686 1.525827

12 C 6.884161 5.377226 4.162566 5.683277 2.529964

13 C 8.121802 6.718856 5.306380 7.159268 3.898892

14 H 2.419993 3.029812 4.459949 3.178792 5.747599

15 H 4.126580 5.666017 6.352835 6.696702 8.128654

16 H 3.017399 2.726196 3.181268 3.232349 4.517043

17 H 3.829268 4.196377 4.783571 4.654600 6.256250

18 H 3.065166 3.544031 3.651221 4.613462 5.358454

19 H 4.424746 2.942434 2.411314 3.333636 1.091998

20 H 4.759247 3.047341 2.409477 3.040576 1.088912

21 H 5.860916 4.541039 2.926243 5.245423 2.161126

22 H 5.590295 4.463764 2.931622 5.403729 2.158261

23 H 6.921581 5.441442 4.463983 5.665015 2.752017

24 H 7.131331 5.495409 4.450642 5.506559 2.747204

25 H 9.023237 7.551994 6.252925 7.820419 4.704133

26 H 8.335339 6.957940 5.423943 7.447698 4.220401

27 H 8.182506 6.936358 5.463791 7.577071 4.239950

11 12 13 14 15

11 C 0.000000

12 C 1.530867 0.000000

13 C 2.546452 1.527223 0.000000

14 H 7.074977 8.255180 9.581735 0.000000

15 H 9.052915 10.508221 11.539524 3.942865 0.000000

16 H 5.560666 6.813794 7.972922 2.462221 4.788510

17 H 7.250077 8.547859 9.653194 2.518167 3.819053

18 H 6.161395 7.593279 8.580427 3.075466 3.537009

19 H 2.163562 2.790013 4.210324 5.926610 8.390307

20 H 2.176125 2.790223 4.215741 5.652205 8.423874

21 H 1.095810 2.156422 2.769579 7.155459 8.971584

22 H 1.096102 2.161352 2.778566 7.364227 8.943193

23 H 2.159160 1.096113 2.158259 8.398023 10.744921

24 H 2.154455 1.096000 2.156181 8.205378 10.756681

25 H 3.499782 2.179412 1.093850 10.417277 12.547230

26 H 2.802417 2.179764 1.094710 9.674665 11.503961

27 H 2.830628 2.178375 1.094549 9.862193 11.529045

16 17 18 19 20

16 H 0.000000

17 H 1.765846 0.000000

18 H 1.772694 1.772700 0.000000

19 H 5.125062 6.829590 5.961786 0.000000

20 H 4.337915 6.102843 5.485552 1.767323 0.000000

21 H 5.326570 6.946889 5.855128 3.068241 2.531408

22 H 5.978975 7.588421 6.305794 2.500529 3.074256

23 H 7.245580 8.994369 8.054745 2.562446 3.101175

24 H 6.707299 8.449647 7.695993 3.113267 2.558457

25 H 8.857011 10.562842 9.569694 4.898524 4.887037

26 H 7.845527 9.460827 8.393971 4.767067 4.444449

27 H 8.339506 9.982289 8.760667 4.434933 4.788439

21 22 23 24 25

21 H 0.000000

22 H 1.755626 0.000000

23 H 3.061178 2.514121 0.000000

24 H 2.502805 3.061389 1.753863 0.000000

25 H 3.767313 3.791428 2.511808 2.489358 0.000000

26 H 2.577161 3.119557 3.078263 2.534236 1.764984

27 H 3.155995 2.618349 2.513926 3.075071 1.764773

26 27

26 H 0.000000

27 H 1.765292 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 8.26D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.105582 -0.431552 -0.068172

2 6 0 -2.811886 0.080624 0.478280

3 8 0 -4.942363 0.255177 -0.621344

4 8 0 -4.253554 -1.763792 0.082463

5 6 0 -2.242125 -0.673487 1.668206

6 16 0 -1.615152 0.085913 -1.008331

7 6 0 -0.128535 0.704058 -0.304679

8 16 0 1.083438 -0.598902 -0.079403

9 16 0 -0.002931 2.280429 0.373229

10 6 0 2.684003 0.301230 -0.071559

11 6 0 3.844861 -0.688784 -0.050860

12 6 0 5.198543 0.025755 -0.027710

13 6 0 6.378018 -0.944093 -0.002355

14 1 0 -2.947775 1.134335 0.718310

15 1 0 -5.109087 -1.997375 -0.314795

16 1 0 -1.308873 -0.201908 1.979653

17 1 0 -2.936338 -0.631594 2.513450

18 1 0 -2.046197 -1.718095 1.431955

19 1 0 2.729686 0.922087 -0.968726

20 1 0 2.701065 0.956400 0.798033

21 1 0 3.765291 -1.340256 0.826666

22 1 0 3.788948 -1.342646 -0.928798

23 1 0 5.279945 0.681466 -0.902285

24 1 0 5.243879 0.678953 0.851206

25 1 0 7.332272 -0.411718 0.047495

26 1 0 6.327845 -1.611726 0.863750

27 1 0 6.397198 -1.570547 -0.899698

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3299377 0.1931612 0.1807078

Leave Link 202 at Sat Aug 17 17:54:03 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.7160185270 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0550068041 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.6610117229 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2342

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.38D-10

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 95

GePol: Fraction of low-weight points (<1% of avg) = 4.06%

GePol: Cavity surface area = 308.238 Ang\*\*2

GePol: Cavity volume = 319.542 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0056630139 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.6553487090 Hartrees.

Leave Link 301 at Sat Aug 17 17:54:03 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.86D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:54:03 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:54:04 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999887 -0.014954 -0.000817 -0.000869 Ang= -1.72 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.63008687214

Leave Link 401 at Sat Aug 17 17:54:04 2019, MaxMem= 1342177280 cpu: 7.7

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16454892.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.22D-15 for 2316.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.53D-15 for 712 256.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.66D-15 for 2316.

Iteration 1 A^-1\*A deviation from orthogonality is 4.11D-13 for 1036 1014.

E= -1658.65097001665

DIIS: error= 5.02D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.65097001665 IErMin= 1 ErrMin= 5.02D-03

ErrMax= 5.02D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.64D-02 BMatP= 5.64D-02

IDIUse=3 WtCom= 9.50D-01 WtEn= 5.02D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.426 Goal= None Shift= 0.000

Gap= 0.486 Goal= None Shift= 0.000

GapD= 0.426 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=5.35D-04 MaxDP=2.01D-02 OVMax= 3.22D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 5.35D-04 CP: 9.99D-01

E= -1658.67627101009 Delta-E= -0.025300993440 Rises=F Damp=F

DIIS: error= 8.08D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67627101009 IErMin= 2 ErrMin= 8.08D-04

ErrMax= 8.08D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.24D-03 BMatP= 5.64D-02

IDIUse=3 WtCom= 9.92D-01 WtEn= 8.08D-03

Coeff-Com: -0.586D-01 0.106D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.581D-01 0.106D+01

Gap= 0.118 Goal= None Shift= 0.000

Gap= 0.137 Goal= None Shift= 0.000

RMSDP=1.19D-04 MaxDP=6.15D-03 DE=-2.53D-02 OVMax= 8.48D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.14D-04 CP: 9.99D-01 1.06D+00

E= -1658.67625114117 Delta-E= 0.000019868914 Rises=F Damp=F

DIIS: error= 1.75D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1658.67627101009 IErMin= 2 ErrMin= 8.08D-04

ErrMax= 1.75D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.25D-03 BMatP= 1.24D-03

IDIUse=3 WtCom= 1.93D-01 WtEn= 8.07D-01

Coeff-Com: -0.488D-01 0.650D+00 0.399D+00

Coeff-En: 0.000D+00 0.517D+00 0.483D+00

Coeff: -0.941D-02 0.542D+00 0.467D+00

Gap= 0.117 Goal= None Shift= 0.000

Gap= 0.137 Goal= None Shift= 0.000

RMSDP=8.76D-05 MaxDP=5.24D-03 DE= 1.99D-05 OVMax= 8.76D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 5.02D-05 CP: 9.99D-01 1.09D+00 3.86D-01

E= -1658.67657818523 Delta-E= -0.000327044055 Rises=F Damp=F

DIIS: error= 9.52D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67657818523 IErMin= 2 ErrMin= 8.08D-04

ErrMax= 9.52D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.93D-04 BMatP= 1.24D-03

IDIUse=3 WtCom= 9.90D-01 WtEn= 9.52D-03

Coeff-Com: -0.136D-01 0.149D+00 0.338D+00 0.527D+00

Coeff-En: 0.000D+00 0.000D+00 0.252D+00 0.748D+00

Coeff: -0.135D-01 0.148D+00 0.337D+00 0.529D+00

Gap= 0.118 Goal= None Shift= 0.000

Gap= 0.137 Goal= None Shift= 0.000

RMSDP=3.09D-05 MaxDP=1.45D-03 DE=-3.27D-04 OVMax= 3.04D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.54D-05 CP: 9.99D-01 1.10D+00 5.67D-01 6.78D-01

E= -1658.67669108004 Delta-E= -0.000112894816 Rises=F Damp=F

DIIS: error= 7.15D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67669108004 IErMin= 5 ErrMin= 7.15D-05

ErrMax= 7.15D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.06D-06 BMatP= 5.93D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.313D-02 0.240D-01 0.127D+00 0.239D+00 0.613D+00

Coeff: -0.313D-02 0.240D-01 0.127D+00 0.239D+00 0.613D+00

Gap= 0.118 Goal= None Shift= 0.000

Gap= 0.137 Goal= None Shift= 0.000

RMSDP=6.22D-06 MaxDP=2.52D-04 DE=-1.13D-04 OVMax= 4.85D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 4.62D-06 CP: 9.99D-01 1.10D+00 5.96D-01 7.17D-01 9.03D-01

E= -1658.67669262652 Delta-E= -0.000001546473 Rises=F Damp=F

DIIS: error= 2.80D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67669262652 IErMin= 6 ErrMin= 2.80D-05

ErrMax= 2.80D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.35D-06 BMatP= 7.06D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.730D-03-0.156D-01 0.111D-01 0.413D-01 0.328D+00 0.634D+00

Coeff: 0.730D-03-0.156D-01 0.111D-01 0.413D-01 0.328D+00 0.634D+00

Gap= 0.118 Goal= None Shift= 0.000

Gap= 0.137 Goal= None Shift= 0.000

RMSDP=2.93D-06 MaxDP=1.19D-04 DE=-1.55D-06 OVMax= 3.95D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.99D-06 CP: 9.99D-01 1.10D+00 6.01D-01 7.50D-01 9.70D-01

CP: 8.62D-01

E= -1658.67669296673 Delta-E= -0.000000340212 Rises=F Damp=F

DIIS: error= 1.10D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67669296673 IErMin= 7 ErrMin= 1.10D-05

ErrMax= 1.10D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.87D-07 BMatP= 1.35D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.701D-03-0.105D-01-0.789D-02-0.456D-02 0.963D-01 0.327D+00

Coeff-Com: 0.599D+00

Coeff: 0.701D-03-0.105D-01-0.789D-02-0.456D-02 0.963D-01 0.327D+00

Coeff: 0.599D+00

Gap= 0.118 Goal= None Shift= 0.000

Gap= 0.137 Goal= None Shift= 0.000

RMSDP=1.37D-06 MaxDP=5.73D-05 DE=-3.40D-07 OVMax= 1.48D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 9.91D-07 CP: 9.99D-01 1.10D+00 6.05D-01 7.53D-01 1.01D+00

CP: 9.63D-01 9.98D-01

E= -1658.67669302014 Delta-E= -0.000000053411 Rises=F Damp=F

DIIS: error= 4.11D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67669302014 IErMin= 8 ErrMin= 4.11D-06

ErrMax= 4.11D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.25D-08 BMatP= 1.87D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.200D-03-0.173D-02-0.700D-02-0.128D-01-0.292D-01 0.263D-01

Coeff-Com: 0.339D+00 0.685D+00

Coeff: 0.200D-03-0.173D-02-0.700D-02-0.128D-01-0.292D-01 0.263D-01

Coeff: 0.339D+00 0.685D+00

Gap= 0.118 Goal= None Shift= 0.000

Gap= 0.137 Goal= None Shift= 0.000

RMSDP=7.68D-07 MaxDP=2.77D-05 DE=-5.34D-08 OVMax= 1.12D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 3.33D-07 CP: 9.99D-01 1.10D+00 6.05D-01 7.58D-01 1.03D+00

CP: 1.04D+00 1.19D+00 8.07D-01

E= -1658.67669303624 Delta-E= -0.000000016105 Rises=F Damp=F

DIIS: error= 2.02D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67669303624 IErMin= 9 ErrMin= 2.02D-06

ErrMax= 2.02D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.10D-08 BMatP= 4.25D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.254D-04 0.121D-02-0.264D-02-0.706D-02-0.377D-01-0.495D-01

Coeff-Com: 0.785D-01 0.410D+00 0.607D+00

Coeff: -0.254D-04 0.121D-02-0.264D-02-0.706D-02-0.377D-01-0.495D-01

Coeff: 0.785D-01 0.410D+00 0.607D+00

Gap= 0.118 Goal= None Shift= 0.000

Gap= 0.137 Goal= None Shift= 0.000

RMSDP=3.43D-07 MaxDP=1.58D-05 DE=-1.61D-08 OVMax= 3.60D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.38D-07 CP: 9.99D-01 1.10D+00 6.06D-01 7.59D-01 1.04D+00

CP: 1.07D+00 1.25D+00 9.83D-01 8.35D-01

E= -1658.67669303961 Delta-E= -0.000000003366 Rises=F Damp=F

DIIS: error= 8.57D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67669303961 IErMin=10 ErrMin= 8.57D-07

ErrMax= 8.57D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.50D-09 BMatP= 1.10D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.513D-04 0.101D-02-0.111D-03-0.155D-02-0.151D-01-0.318D-01

Coeff-Com: -0.236D-01 0.975D-01 0.327D+00 0.647D+00

Coeff: -0.513D-04 0.101D-02-0.111D-03-0.155D-02-0.151D-01-0.318D-01

Coeff: -0.236D-01 0.975D-01 0.327D+00 0.647D+00

Gap= 0.118 Goal= None Shift= 0.000

Gap= 0.137 Goal= None Shift= 0.000

RMSDP=1.13D-07 MaxDP=5.12D-06 DE=-3.37D-09 OVMax= 2.21D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 5.13D-08 CP: 9.99D-01 1.10D+00 6.07D-01 7.60D-01 1.04D+00

CP: 1.08D+00 1.29D+00 1.02D+00 9.59D-01 8.67D-01

E= -1658.67669304011 Delta-E= -0.000000000500 Rises=F Damp=F

DIIS: error= 1.57D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67669304011 IErMin=11 ErrMin= 1.57D-07

ErrMax= 1.57D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.46D-11 BMatP= 1.50D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.110D-04 0.147D-03 0.199D-03 0.189D-03-0.428D-03-0.353D-02

Coeff-Com: -0.148D-01-0.140D-01 0.157D-01 0.190D+00 0.827D+00

Coeff: -0.110D-04 0.147D-03 0.199D-03 0.189D-03-0.428D-03-0.353D-02

Coeff: -0.148D-01-0.140D-01 0.157D-01 0.190D+00 0.827D+00

Gap= 0.118 Goal= None Shift= 0.000

Gap= 0.137 Goal= None Shift= 0.000

RMSDP=4.18D-08 MaxDP=1.85D-06 DE=-5.00D-10 OVMax= 4.89D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.96D-08 CP: 9.99D-01 1.10D+00 6.07D-01 7.60D-01 1.04D+00

CP: 1.08D+00 1.29D+00 1.04D+00 1.00D+00 1.01D+00

CP: 1.10D+00

E= -1658.67669304016 Delta-E= -0.000000000053 Rises=F Damp=F

DIIS: error= 9.00D-08 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.67669304016 IErMin=12 ErrMin= 9.00D-08

ErrMax= 9.00D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.17D-11 BMatP= 8.46D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.189D-05-0.731D-04 0.110D-03 0.309D-03 0.195D-02 0.291D-02

Coeff-Com: -0.321D-02-0.189D-01-0.401D-01 0.690D-02 0.402D+00 0.649D+00

Coeff: 0.189D-05-0.731D-04 0.110D-03 0.309D-03 0.195D-02 0.291D-02

Coeff: -0.321D-02-0.189D-01-0.401D-01 0.690D-02 0.402D+00 0.649D+00

Gap= 0.118 Goal= None Shift= 0.000

Gap= 0.137 Goal= None Shift= 0.000

RMSDP=1.40D-08 MaxDP=6.85D-07 DE=-5.28D-11 OVMax= 2.09D-06

Cycle 13 Pass 1 IDiag 1:

RMSU= 7.96D-09 CP: 9.99D-01 1.10D+00 6.07D-01 7.60D-01 1.04D+00

CP: 1.08D+00 1.29D+00 1.04D+00 1.01D+00 1.05D+00

CP: 1.25D+00 8.68D-01

E= -1658.67669304018 Delta-E= -0.000000000018 Rises=F Damp=F

DIIS: error= 2.50D-08 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1658.67669304018 IErMin=13 ErrMin= 2.50D-08

ErrMax= 2.50D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.26D-12 BMatP= 2.17D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.248D-05-0.490D-04 0.206D-05 0.719D-04 0.694D-03 0.151D-02

Coeff-Com: 0.154D-02-0.350D-02-0.176D-01-0.309D-01-0.216D-01 0.210D+00

Coeff-Com: 0.860D+00

Coeff: 0.248D-05-0.490D-04 0.206D-05 0.719D-04 0.694D-03 0.151D-02

Coeff: 0.154D-02-0.350D-02-0.176D-01-0.309D-01-0.216D-01 0.210D+00

Coeff: 0.860D+00

Gap= 0.118 Goal= None Shift= 0.000

Gap= 0.137 Goal= None Shift= 0.000

RMSDP=7.47D-09 MaxDP=3.82D-07 DE=-1.77D-11 OVMax= 9.87D-07

Error on total polarization charges = 0.04161

SCF Done: E(UB3LYP) = -1658.67669304 A.U. after 13 cycles

NFock= 13 Conv=0.75D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655239901750D+03 PE=-6.148072152711D+03 EE= 1.731500209212D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.55

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:54:32 2019, MaxMem= 1342177280 cpu: 327.4

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 339

Leave Link 701 at Sat Aug 17 17:54:33 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:54:33 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:54:37 2019, MaxMem= 1342177280 cpu: 38.4

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.49977665D+00-2.96886488D+00 7.01404387D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.004533160 0.005198599 -0.000263531

2 6 0.002475250 0.000887108 0.001578539

3 8 0.003586411 -0.004771517 0.001397158

4 8 -0.001804982 -0.000146421 -0.000698584

5 6 -0.000025668 0.001810087 -0.001434656

6 16 0.000655085 0.000424987 0.000609421

7 6 -0.001018546 -0.000729092 -0.000595224

8 16 0.000700663 0.000016161 0.000710414

9 16 0.000967111 0.000126935 -0.000111619

10 6 -0.000288666 -0.001029789 -0.001593579

11 6 -0.000404870 0.000325716 0.000231920

12 6 0.000357106 -0.000423742 0.000779012

13 6 0.000069094 -0.000023484 -0.000422783

14 1 -0.000751093 -0.000256380 -0.000269283

15 1 -0.000166504 -0.001312109 -0.000424114

16 1 0.000115677 -0.000657831 -0.000099083

17 1 -0.000252873 -0.000046160 -0.000068016

18 1 0.000427288 -0.000776487 -0.000255507

19 1 -0.001048821 0.000538495 0.000049698

20 1 0.000845543 0.000459246 0.000497963

21 1 -0.000031257 -0.000144271 0.000417430

22 1 0.000309513 0.000220272 -0.000058075

23 1 -0.000147082 0.000065880 -0.000107880

24 1 -0.000030832 0.000269046 0.000186648

25 1 0.000152412 0.000190394 -0.000026332

26 1 -0.000100137 -0.000006857 0.000192730

27 1 -0.000056663 -0.000208784 -0.000222666

-------------------------------------------------------------------

Cartesian Forces: Max 0.005198599 RMS 0.001222083

Leave Link 716 at Sat Aug 17 17:54:37 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.005913730 RMS 0.000865467

Search for a local minimum.

Step number 53 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .86547D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 3 4 5 6

2 8 9 10 11

12 13 14 15 16

17 18 20 21 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43 45 44 47 46

49 48 51 50 52

53

ITU= 0 0 0 0 0 0 0 0 0 1 1 1 1 1 -1 -1 0 -1 -1 -1

ITU= 0 -1 0 0 -1 -1 0 0 -1 0 0 -1 1 -1 1 -1 1 1 -1 1

ITU= -1 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Eigenvalues --- -0.00237 0.00000 0.00002 0.00082 0.00151

Eigenvalues --- 0.00247 0.00311 0.00474 0.01400 0.01502

Eigenvalues --- 0.02026 0.02770 0.03488 0.03606 0.04105

Eigenvalues --- 0.04371 0.04686 0.04820 0.04926 0.05312

Eigenvalues --- 0.05424 0.05486 0.05618 0.05823 0.06367

Eigenvalues --- 0.07956 0.08352 0.09160 0.10657 0.11306

Eigenvalues --- 0.12138 0.13381 0.14184 0.15025 0.15648

Eigenvalues --- 0.15950 0.16083 0.16283 0.16618 0.17296

Eigenvalues --- 0.17878 0.19749 0.21062 0.21790 0.22302

Eigenvalues --- 0.22763 0.23088 0.25024 0.25347 0.26756

Eigenvalues --- 0.27154 0.28606 0.29212 0.29453 0.29813

Eigenvalues --- 0.30088 0.32256 0.33261 0.33712 0.33878

Eigenvalues --- 0.33890 0.33959 0.33990 0.34034 0.34070

Eigenvalues --- 0.34159 0.34184 0.34501 0.34516 0.34862

Eigenvalues --- 0.35497 0.35780 0.46909 0.52197 0.85015

Eigenvalue 1 is -2.37D-03 should be greater than 0.000000 Eigenvector:

D24 D4 D6 D5 D22

1 -0.36828 -0.29844 -0.27704 -0.25514 0.24654

D1 D20 D19 D18 D3

1 -0.23562 -0.22926 -0.22584 -0.21910 -0.21422

Eigenvalue 2 is 1.86D-06 Eigenvector:

D23 D24 D26 D54 D51

1 0.34249 0.31603 0.20857 -0.20472 -0.19560

D25 D48 D1 D53 D52

1 0.19314 -0.19173 -0.18346 -0.18098 -0.17995

Eigenvalue 3 is 1.57D-05 Eigenvector:

D25 D26 D27 D2 D5

1 0.35766 0.34355 0.34013 0.24988 0.21296

D1 D3 D22 D4 D6

1 0.21180 0.19363 0.18348 0.17488 0.15671

Use linear search instead of GDIIS.

RFO step: Lambda=-2.37263729D-03 EMin=-2.37253298D-03

I= 1 Eig= -2.37D-03 Dot1= 4.73D-06

I= 1 Stepn= 2.99D-01 RXN= 2.99D-01 EDone=F

Mixed 1 eigenvectors in step. Raw Step.Grad= 4.73D-06.

RFO eigenvector is Hessian eigenvector with negative curvature.

Taking step of 2.99D-01 in eigenvector direction(s). Step.Grad= -4.82D-06.

Quartic linear search produced a step of -0.98201.

Iteration 1 RMS(Cart)= 0.13112682 RMS(Int)= 0.00633098

Iteration 2 RMS(Cart)= 0.01502294 RMS(Int)= 0.00006528

Iteration 3 RMS(Cart)= 0.00012322 RMS(Int)= 0.00005312

Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00005312

ITry= 1 IFail=0 DXMaxC= 5.17D-01 DCOld= 1.00D+10 DXMaxT= 1.20D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.82486 0.00283 0.01066 0.00222 0.01288 2.83774

R2 2.29724 -0.00591 -0.00779 0.00056 -0.00723 2.29002

R3 2.54900 0.00162 0.00409 0.00480 0.00889 2.55789

R4 2.87166 -0.00145 -0.00646 0.00208 -0.00438 2.86728

R5 3.60646 0.00012 0.00412 -0.02702 -0.02290 3.58357

R6 2.05832 -0.00023 -0.00024 0.00195 0.00170 2.06002

R7 1.83636 0.00060 0.00057 0.00342 0.00398 1.84034

R8 2.06175 -0.00021 -0.00050 0.00075 0.00025 2.06200

R9 2.06847 0.00011 0.00015 0.00103 0.00117 2.06965

R10 2.05747 0.00089 0.00253 0.00483 0.00737 2.06484

R11 3.32036 0.00012 -0.00511 0.01987 0.01475 3.33512

R12 3.38959 0.00012 -0.00190 0.00190 0.00000 3.38959

R13 3.25136 0.00014 0.00245 -0.00050 0.00195 3.25331

R14 3.47016 -0.00025 0.00209 -0.00137 0.00071 3.47088

R15 2.88339 -0.00009 -0.00199 -0.00093 -0.00292 2.88048

R16 2.06358 0.00026 0.00067 0.00137 0.00204 2.06562

R17 2.05775 0.00068 0.00229 0.00363 0.00592 2.06366

R18 2.89292 0.00015 0.00119 0.00330 0.00449 2.89741

R19 2.07078 0.00041 0.00139 0.00249 0.00388 2.07466

R20 2.07133 -0.00007 -0.00019 0.00081 0.00062 2.07195

R21 2.88603 0.00012 0.00019 0.00249 0.00268 2.88871

R22 2.07135 0.00010 0.00055 0.00150 0.00205 2.07340

R23 2.07114 0.00030 0.00065 0.00175 0.00239 2.07353

R24 2.06708 0.00022 0.00056 0.00125 0.00180 2.06888

R25 2.06870 0.00015 0.00052 0.00097 0.00149 2.07019

R26 2.06840 0.00030 0.00065 0.00099 0.00165 2.07005

A1 2.17548 0.00100 0.00077 0.01068 0.01135 2.18683

A2 1.97416 0.00115 0.00328 -0.00586 -0.00269 1.97148

A3 2.13323 -0.00216 -0.00431 -0.00526 -0.00967 2.12356

A4 2.02718 -0.00030 0.00029 -0.02066 -0.02030 2.00688

A5 1.83266 0.00128 -0.00357 0.03312 0.02959 1.86226

A6 1.87973 -0.00059 -0.00583 -0.00249 -0.00828 1.87145

A7 1.95651 -0.00159 -0.00963 0.00064 -0.00887 1.94764

A8 1.93295 0.00093 0.00811 0.00805 0.01608 1.94903

A9 1.82060 0.00034 0.01129 -0.01794 -0.00661 1.81399

A10 1.86328 0.00216 0.00888 0.01197 0.02086 1.88414

A11 1.90683 0.00068 0.00598 0.00109 0.00707 1.91390

A12 1.92611 -0.00027 0.00026 0.00218 0.00243 1.92854

A13 1.95377 -0.00005 -0.00136 0.00024 -0.00112 1.95266

A14 1.88129 0.00004 0.00213 0.00162 0.00372 1.88501

A15 1.89939 -0.00049 -0.00502 -0.00361 -0.00863 1.89076

A16 1.89485 0.00008 -0.00200 -0.00156 -0.00356 1.89129

A17 1.79218 0.00180 0.00650 -0.01276 -0.00625 1.78592

A18 1.94596 0.00159 0.02375 0.00453 0.02837 1.97433

A19 2.14347 0.00075 -0.00053 -0.00443 -0.00491 2.13856

A20 2.17333 -0.00212 -0.01787 -0.01020 -0.02796 2.14536

A21 1.80637 -0.00194 -0.01062 -0.00841 -0.01903 1.78734

A22 1.92318 0.00040 0.00327 -0.00654 -0.00325 1.91993

A23 1.88772 -0.00086 -0.00843 -0.01341 -0.02175 1.86597

A24 1.88809 0.00047 0.00394 0.01238 0.01633 1.90442

A25 1.92646 0.00119 0.01259 0.01103 0.02363 1.95009

A26 1.94726 -0.00100 -0.00896 -0.00208 -0.01104 1.93622

A27 1.88953 -0.00022 -0.00268 -0.00167 -0.00431 1.88523

A28 1.94992 0.00044 0.00301 0.00772 0.01073 1.96065

A29 1.91916 -0.00007 -0.00306 -0.00027 -0.00335 1.91581

A30 1.91493 -0.00009 0.00211 -0.00583 -0.00370 1.91123

A31 1.90667 -0.00021 0.00028 -0.00047 -0.00019 1.90647

A32 1.91310 -0.00027 -0.00456 -0.00270 -0.00725 1.90585

A33 1.85778 0.00018 0.00214 0.00122 0.00335 1.86113

A34 1.96791 -0.00010 -0.00183 -0.00326 -0.00513 1.96277

A35 1.91009 -0.00014 -0.00388 -0.00496 -0.00888 1.90121

A36 1.90380 0.00009 0.00400 0.00709 0.01110 1.91490

A37 1.91323 0.00000 -0.00041 -0.00341 -0.00389 1.90935

A38 1.91051 0.00019 0.00229 0.00362 0.00590 1.91641

A39 1.85485 -0.00004 -0.00006 0.00125 0.00122 1.85607

A40 1.94488 -0.00007 0.00063 -0.00350 -0.00287 1.94201

A41 1.94446 -0.00019 -0.00231 -0.00289 -0.00521 1.93926

A42 1.94269 0.00003 0.00014 -0.00111 -0.00098 1.94171

A43 1.87628 0.00012 0.00064 0.00367 0.00430 1.88058

A44 1.87615 0.00005 0.00095 0.00376 0.00471 1.88086

A45 1.87588 0.00006 0.00006 0.00057 0.00062 1.87650

D1 2.63074 0.00106 0.08537 -0.07050 0.01504 2.64579

D2 -1.48061 -0.00020 0.07037 -0.05754 0.01283 -1.46779

D3 0.45224 0.00051 0.07913 -0.06409 0.01500 0.46724

D4 -0.53694 0.00043 0.07568 -0.08929 -0.01353 -0.55047

D5 1.63489 -0.00083 0.06068 -0.07634 -0.01575 1.61914

D6 -2.71545 -0.00012 0.06944 -0.08289 -0.01357 -2.72902

D7 -3.12412 0.00063 0.02337 0.00819 0.03142 -3.09270

D8 -0.00790 0.00007 0.01406 -0.00982 0.00437 -0.00353

D9 -3.13183 -0.00002 -0.01208 0.04907 0.03703 -3.09480

D10 -1.06630 0.00029 -0.00564 0.05301 0.04744 -1.01887

D11 1.04625 0.00016 -0.00893 0.05271 0.04384 1.09009

D12 1.04465 -0.00023 0.00023 0.01959 0.01979 1.06444

D13 3.11018 0.00008 0.00667 0.02354 0.03019 3.14037

D14 -1.06045 -0.00004 0.00339 0.02323 0.02659 -1.03386

D15 -0.98081 -0.00027 -0.01298 0.03640 0.02338 -0.95743

D16 1.08472 0.00004 -0.00654 0.04035 0.03379 1.11851

D17 -3.08592 -0.00008 -0.00982 0.04004 0.03019 -3.05573

D18 3.13516 0.00009 0.05934 -0.06555 -0.00617 3.12900

D19 -0.93214 -0.00040 0.05114 -0.06757 -0.01648 -0.94862

D20 1.16021 0.00010 0.06270 -0.06859 -0.00590 1.15432

D21 1.84225 -0.00036 -0.01919 0.02212 0.00276 1.84501

D22 -1.09224 -0.00118 -0.04638 0.07376 0.02756 -1.06468

D23 2.72152 -0.00094 -0.12655 -0.05836 -0.18507 2.53646

D24 -0.63139 0.00031 -0.09665 -0.11019 -0.20668 -0.83808

D25 -3.02599 -0.00052 -0.00461 0.01910 0.01445 -3.01154

D26 -0.91876 0.00065 0.00747 0.02031 0.02785 -0.89092

D27 1.12421 0.00017 0.00189 0.01778 0.01964 1.14384

D28 -3.13028 -0.00002 0.00577 -0.00672 -0.00098 -3.13126

D29 -1.01012 -0.00004 0.00602 -0.00232 0.00367 -1.00645

D30 1.02752 0.00009 0.00807 -0.00443 0.00362 1.03113

D31 1.06908 0.00004 0.00614 0.00708 0.01324 1.08232

D32 -3.09395 0.00002 0.00640 0.01147 0.01789 -3.07606

D33 -1.05631 0.00015 0.00844 0.00937 0.01784 -1.03847

D34 -1.03262 0.00018 0.00703 0.00312 0.01015 -1.02247

D35 1.08754 0.00016 0.00728 0.00751 0.01479 1.10234

D36 3.12518 0.00029 0.00933 0.00540 0.01474 3.13992

D37 3.13851 0.00025 0.01198 0.01376 0.02574 -3.11893

D38 -1.01037 0.00008 0.00745 0.00360 0.01108 -0.99929

D39 1.01218 0.00000 0.00745 0.00631 0.01376 1.02594

D40 1.01114 0.00019 0.01367 0.00934 0.02299 1.03413

D41 -3.13774 0.00002 0.00914 -0.00082 0.00833 -3.12941

D42 -1.11519 -0.00005 0.00914 0.00189 0.01101 -1.10418

D43 -1.01823 0.00024 0.01351 0.00967 0.02316 -0.99507

D44 1.11607 0.00008 0.00898 -0.00049 0.00851 1.12457

D45 3.13862 0.00000 0.00898 0.00222 0.01118 -3.13338

D46 -3.10857 -0.00016 -0.03730 0.00010 -0.03720 3.13742

D47 -1.01306 -0.00019 -0.03763 0.00043 -0.03720 -1.05026

D48 1.08047 -0.00021 -0.03903 -0.00156 -0.04057 1.03989

D49 1.04208 0.00009 -0.03079 0.01115 -0.01966 1.02242

D50 3.13759 0.00006 -0.03113 0.01147 -0.01966 3.11793

D51 -1.05207 0.00004 -0.03252 0.00949 -0.02304 -1.07510

D52 -0.98604 0.00003 -0.03180 0.00952 -0.02227 -1.00831

D53 1.10948 0.00000 -0.03213 0.00985 -0.02228 1.08720

D54 -3.08018 -0.00002 -0.03352 0.00787 -0.02565 -3.10583

Item Value Threshold Converged?

Maximum Force 0.005914 0.000450 NO

RMS Force 0.000865 0.000300 NO

Maximum Displacement 0.517136 0.001800 NO

RMS Displacement 0.135004 0.001200 NO

Predicted change in Energy=-4.101555D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:54:37 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.114136 -0.362184 -0.203889

2 6 0 -2.827674 0.059137 0.446116

3 8 0 -4.913161 0.385386 -0.724673

4 8 0 -4.283476 -1.705052 -0.218018

5 6 0 -2.345746 -0.849316 1.561756

6 16 0 -1.540443 0.207093 -0.938535

7 6 0 -0.099197 0.721994 -0.059646

8 16 0 1.116065 -0.584009 0.126969

9 16 0 -0.033832 2.194855 0.829311

10 6 0 2.702648 0.335385 0.022252

11 6 0 3.870431 -0.643243 -0.022499

12 6 0 5.225789 0.069817 -0.095866

13 6 0 6.397282 -0.909171 -0.172836

14 1 0 -2.961029 1.084551 0.791217

15 1 0 -5.111939 -1.898171 -0.692114

16 1 0 -1.435632 -0.438878 2.002062

17 1 0 -3.101295 -0.920938 2.351376

18 1 0 -2.128486 -1.857475 1.200745

19 1 0 2.654952 0.950135 -0.880315

20 1 0 2.786179 1.003563 0.881973

21 1 0 3.848689 -1.288148 0.865718

22 1 0 3.762420 -1.302592 -0.891835

23 1 0 5.237511 0.722189 -0.977975

24 1 0 5.346415 0.726099 0.775188

25 1 0 7.354065 -0.379975 -0.228674

26 1 0 6.426374 -1.559731 0.708094

27 1 0 6.319385 -1.552960 -1.055681

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.501667 0.000000

3 O 1.211824 2.413802 0.000000

4 O 1.353577 2.381764 2.241235 0.000000

5 C 2.545978 1.517299 3.652926 2.766709 0.000000

6 S 2.736363 1.896342 3.384192 3.420479 2.831248

7 C 4.161249 2.853027 4.871326 4.839818 3.185112

8 S 5.245348 4.008562 6.165759 5.525468 3.756745

9 S 4.924920 3.537468 5.431104 5.862222 3.892094

10 C 6.856113 5.553416 7.652512 7.281967 5.409238

11 C 7.991572 6.751115 8.871450 8.225076 6.418192

12 C 9.350535 8.071687 10.163331 9.674255 7.805168

13 C 10.525687 9.296265 11.397655 10.710466 8.913637

14 H 2.100698 1.090116 2.568574 3.247970 2.170748

15 H 1.895582 3.216285 2.292424 0.973865 3.719120

16 H 3.470805 2.146338 4.495298 3.826509 1.091162

17 H 2.804895 2.159962 3.801503 2.934991 1.095210

18 H 2.855118 2.175254 4.061043 2.584590 1.092665

19 H 6.928224 5.710734 7.590751 7.458582 5.848821

20 H 7.117493 5.709401 7.889442 7.650268 5.498356

21 H 8.087525 6.823860 9.060909 8.214646 6.248845

22 H 7.962272 6.861031 8.839848 8.084086 6.598125

23 H 9.446078 8.216744 10.159416 9.854858 8.150193

24 H 9.573138 8.207853 10.374226 9.981571 7.891131

25 H 11.468242 10.213518 12.301082 11.712741 9.874828

26 H 10.647450 9.398233 11.594023 10.750800 8.842144

27 H 10.535742 9.408663 11.403370 10.636986 9.079129

6 7 8 9 10

6 S 0.000000

7 C 1.764868 0.000000

8 S 2.969541 1.793692 0.000000

9 S 3.057180 1.721579 3.088305 0.000000

10 C 4.352400 2.829577 1.836708 3.405479 0.000000

11 C 5.553355 4.197999 2.759055 4.901392 1.524282

12 C 6.819885 5.364897 4.167371 5.747638 2.539827

13 C 8.052317 6.699086 5.299705 7.210999 3.903499

14 H 2.404171 3.007574 4.455111 3.130928 5.764528

15 H 4.153126 5.691474 6.417628 6.697370 8.158852

16 H 3.012536 2.717411 3.169889 3.205766 4.652364

17 H 3.812116 4.186269 4.779919 4.629706 6.378786

18 H 3.030636 3.515716 3.647166 4.576780 5.434826

19 H 4.261084 2.882860 2.395077 3.420775 1.093078

20 H 4.761120 3.048167 2.424809 3.061766 1.092043

21 H 5.876548 4.525790 2.916984 5.215995 2.158867

22 H 5.513772 4.438870 2.925323 5.441140 2.154447

23 H 6.797612 5.415143 4.462440 5.763860 2.752382

24 H 7.115829 5.509233 4.475761 5.577385 2.776522

25 H 8.942081 7.536180 6.251460 7.894941 4.712790

26 H 8.324856 6.955485 5.430389 7.473009 4.234145

27 H 8.055334 6.882274 5.423289 7.613322 4.220021

11 12 13 14 15

11 C 0.000000

12 C 1.533243 0.000000

13 C 2.545250 1.528640 0.000000

14 H 7.093395 8.297023 9.616773 0.000000

15 H 9.094295 10.540262 11.563302 3.965264 0.000000

16 H 5.682862 7.002471 8.142844 2.472614 4.785745

17 H 7.370031 8.735612 9.828263 2.544752 3.776309

18 H 6.241610 7.712394 8.687620 3.084860 3.533492

19 H 2.179929 2.828343 4.238229 5.861001 8.274833

20 H 2.169249 2.789219 4.220336 5.748495 8.560262

21 H 1.097864 2.159889 2.778048 7.211623 9.115472

22 H 1.096427 2.158362 2.759391 7.330476 8.896564

23 H 2.155515 1.097198 2.157465 8.395082 10.679847

24 H 2.165625 1.097265 2.162679 8.315189 10.881955

25 H 3.499646 2.179337 1.094805 10.468341 12.566660

26 H 2.811861 2.177885 1.095497 9.753075 11.627889

27 H 2.809346 2.179588 1.095421 9.823115 11.442313

16 17 18 19 20

16 H 0.000000

17 H 1.768851 0.000000

18 H 1.770473 1.774094 0.000000

19 H 5.193297 6.861422 5.924083 0.000000

20 H 4.599883 6.365940 5.695708 1.767974 0.000000

21 H 5.471434 7.116480 6.013568 3.079538 2.526090

22 H 6.011687 7.600964 6.276110 2.510259 3.068842

23 H 7.399969 9.127986 8.103049 2.594438 3.089920

24 H 6.989889 8.749908 7.920234 3.167784 2.577440

25 H 9.068540 10.782571 9.702835 4.927016 4.900336

26 H 8.046230 9.689422 8.574205 4.800635 4.455528

27 H 8.410188 10.037763 8.749326 4.441206 4.772196

21 22 23 24 25

21 H 0.000000

22 H 1.759728 0.000000

23 H 3.060962 2.506603 0.000000

24 H 2.511687 3.066528 1.756547 0.000000

25 H 3.782873 3.767084 2.501204 2.502358 0.000000

26 H 2.596741 3.118100 3.076262 2.528998 1.769171

27 H 3.141057 2.574413 2.520475 3.081049 1.769293

26 27

26 H 0.000000

27 H 1.767030 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.23D-01

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.123009 -0.421950 -0.144998

2 6 0 -2.832141 0.116136 0.401925

3 8 0 -4.926990 0.211815 -0.793439

4 8 0 -4.290697 -1.742491 0.100403

5 6 0 -2.340465 -0.561188 1.667501

6 16 0 -1.555785 -0.004891 -0.995351

7 6 0 -0.108500 0.668969 -0.242994

8 16 0 1.109866 -0.577101 0.181533

9 16 0 -0.038230 2.285148 0.345955

10 6 0 2.694393 0.304750 -0.110199

11 6 0 3.863077 -0.664476 0.024764

12 6 0 5.216898 0.020950 -0.194767

13 6 0 6.389043 -0.954819 -0.091382

14 1 0 -2.964180 1.188771 0.544660

15 1 0 -5.122527 -2.022923 -0.321297

16 1 0 -1.427532 -0.073991 2.013661

17 1 0 -3.089828 -0.479652 2.462039

18 1 0 -2.124669 -1.619961 1.505184

19 1 0 2.638958 0.734686 -1.113644

20 1 0 2.783657 1.125611 0.604487

21 1 0 3.849005 -1.126749 1.020461

22 1 0 3.749249 -1.478517 -0.700862

23 1 0 5.220986 0.491725 -1.185825

24 1 0 5.343357 0.832308 0.533036

25 1 0 7.344676 -0.446390 -0.255286

26 1 0 6.425756 -1.424051 0.897854

27 1 0 6.305205 -1.756190 -0.833489

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3356436 0.1917516 0.1799562

Leave Link 202 at Sat Aug 17 17:54:37 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1101.5708588998 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0550299180 Hartrees.

Nuclear repulsion after empirical dispersion term = 1101.5158289818 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2298

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.13D-09

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 82

GePol: Fraction of low-weight points (<1% of avg) = 3.57%

GePol: Cavity surface area = 308.879 Ang\*\*2

GePol: Cavity volume = 320.170 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0056491658 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1101.5101798160 Hartrees.

Leave Link 301 at Sat Aug 17 17:54:37 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.86D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:54:37 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:54:37 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Lowest energy guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999959 0.008958 0.000868 -0.001085 Ang= 1.04 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999697 0.024540 0.001716 -0.000221 Ang= 2.82 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 1.80D-02

Max alpha theta= 3.595 degrees.

Max beta theta= 3.643 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7553 S= 0.5026

Leave Link 401 at Sat Aug 17 17:54:38 2019, MaxMem= 1342177280 cpu: 4.3

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 15842412.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.33D-15 for 2289.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.12D-15 for 1838 1650.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.55D-15 for 2289.

Iteration 1 A^-1\*A deviation from orthogonality is 5.38D-12 for 593 574.

E= -1658.66473578494

DIIS: error= 3.62D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.66473578494 IErMin= 1 ErrMin= 3.62D-03

ErrMax= 3.62D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.45D-02 BMatP= 2.45D-02

IDIUse=3 WtCom= 9.64D-01 WtEn= 3.62D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 88.671 Goal= None Shift= 0.000

Gap= 88.662 Goal= None Shift= 0.000

GapD= 88.662 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=4.27D-04 MaxDP=1.60D-02 OVMax= 2.75D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.27D-04 CP: 9.99D-01

E= -1658.67639446850 Delta-E= -0.011658683555 Rises=F Damp=F

DIIS: error= 3.73D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67639446850 IErMin= 2 ErrMin= 3.73D-04

ErrMax= 3.73D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.64D-04 BMatP= 2.45D-02

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.73D-03

Coeff-Com: -0.593D-01 0.106D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.591D-01 0.106D+01

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=8.00D-05 MaxDP=3.93D-03 DE=-1.17D-02 OVMax= 7.28D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 7.72D-05 CP: 9.99D-01 1.05D+00

E= -1658.67652517068 Delta-E= -0.000130702179 Rises=F Damp=F

DIIS: error= 4.34D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67652517068 IErMin= 2 ErrMin= 3.73D-04

ErrMax= 4.34D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.30D-04 BMatP= 4.64D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 4.34D-03

Coeff-Com: -0.338D-01 0.454D+00 0.579D+00

Coeff-En: 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.336D-01 0.452D+00 0.581D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.67D-05 MaxDP=1.58D-03 DE=-1.31D-04 OVMax= 2.31D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.36D-05 CP: 9.99D-01 1.08D+00 6.92D-01

E= -1658.67656593805 Delta-E= -0.000040767367 Rises=F Damp=F

DIIS: error= 3.35D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67656593805 IErMin= 4 ErrMin= 3.35D-04

ErrMax= 3.35D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.36D-05 BMatP= 2.30D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.35D-03

Coeff-Com: -0.149D-01 0.183D+00 0.374D+00 0.458D+00

Coeff-En: 0.000D+00 0.000D+00 0.179D+00 0.821D+00

Coeff: -0.148D-01 0.183D+00 0.373D+00 0.459D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.41D-05 MaxDP=7.71D-04 DE=-4.08D-05 OVMax= 1.44D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.18D-05 CP: 9.99D-01 1.09D+00 7.56D-01 7.84D-01

E= -1658.67657958145 Delta-E= -0.000013643400 Rises=F Damp=F

DIIS: error= 8.50D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67657958145 IErMin= 5 ErrMin= 8.50D-05

ErrMax= 8.50D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.16D-06 BMatP= 7.36D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.285D-02 0.275D-01 0.120D+00 0.264D+00 0.591D+00

Coeff: -0.285D-02 0.275D-01 0.120D+00 0.264D+00 0.591D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.69D-06 MaxDP=1.75D-04 DE=-1.36D-05 OVMax= 4.07D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.36D-06 CP: 9.99D-01 1.09D+00 7.89D-01 8.57D-01 9.11D-01

E= -1658.67658096219 Delta-E= -0.000001380739 Rises=F Damp=F

DIIS: error= 1.26D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67658096219 IErMin= 6 ErrMin= 1.26D-05

ErrMax= 1.26D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.67D-07 BMatP= 6.16D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.885D-03-0.162D-01 0.116D-02 0.573D-01 0.259D+00 0.698D+00

Coeff: 0.885D-03-0.162D-01 0.116D-02 0.573D-01 0.259D+00 0.698D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.26D-06 MaxDP=1.03D-04 DE=-1.38D-06 OVMax= 2.83D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.42D-06 CP: 9.99D-01 1.09D+00 8.05D-01 9.00D-01 9.69D-01

CP: 9.42D-01

E= -1658.67658112793 Delta-E= -0.000000165749 Rises=F Damp=F

DIIS: error= 4.52D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67658112793 IErMin= 7 ErrMin= 4.52D-06

ErrMax= 4.52D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.51D-08 BMatP= 4.67D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.647D-03-0.898D-02-0.141D-01-0.113D-01 0.158D-01 0.253D+00

Coeff-Com: 0.765D+00

Coeff: 0.647D-03-0.898D-02-0.141D-01-0.113D-01 0.158D-01 0.253D+00

Coeff: 0.765D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.32D-06 MaxDP=5.38D-05 DE=-1.66D-07 OVMax= 2.21D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 6.81D-07 CP: 9.99D-01 1.09D+00 8.11D-01 9.14D-01 1.03D+00

CP: 1.08D+00 1.19D+00

E= -1658.67658115250 Delta-E= -0.000000024563 Rises=F Damp=F

DIIS: error= 3.41D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67658115250 IErMin= 8 ErrMin= 3.41D-06

ErrMax= 3.41D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.73D-08 BMatP= 5.51D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.221D-03-0.213D-02-0.905D-02-0.184D-01-0.440D-01 0.965D-02

Coeff-Com: 0.465D+00 0.599D+00

Coeff: 0.221D-03-0.213D-02-0.905D-02-0.184D-01-0.440D-01 0.965D-02

Coeff: 0.465D+00 0.599D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.99D-07 MaxDP=2.39D-05 DE=-2.46D-08 OVMax= 6.03D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.63D-07 CP: 9.99D-01 1.09D+00 8.13D-01 9.22D-01 1.04D+00

CP: 1.15D+00 1.33D+00 7.43D-01

E= -1658.67658116135 Delta-E= -0.000000008849 Rises=F Damp=F

DIIS: error= 1.84D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67658116135 IErMin= 9 ErrMin= 1.84D-06

ErrMax= 1.84D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.52D-09 BMatP= 2.73D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.339D-04 0.112D-02-0.180D-02-0.806D-02-0.302D-01-0.563D-01

Coeff-Com: 0.850D-01 0.364D+00 0.646D+00

Coeff: -0.339D-04 0.112D-02-0.180D-02-0.806D-02-0.302D-01-0.563D-01

Coeff: 0.850D-01 0.364D+00 0.646D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.74D-07 MaxDP=1.13D-05 DE=-8.85D-09 OVMax= 3.67D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.18D-07 CP: 9.99D-01 1.09D+00 8.14D-01 9.23D-01 1.05D+00

CP: 1.17D+00 1.43D+00 9.00D-01 7.97D-01

E= -1658.67658116316 Delta-E= -0.000000001813 Rises=F Damp=F

DIIS: error= 5.44D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67658116316 IErMin=10 ErrMin= 5.44D-07

ErrMax= 5.44D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.88D-10 BMatP= 5.52D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.538D-04 0.965D-03 0.378D-03-0.171D-02-0.970D-02-0.325D-01

Coeff-Com: -0.272D-01 0.112D+00 0.356D+00 0.602D+00

Coeff: -0.538D-04 0.965D-03 0.378D-03-0.171D-02-0.970D-02-0.325D-01

Coeff: -0.272D-01 0.112D+00 0.356D+00 0.602D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=8.01D-08 MaxDP=4.71D-06 DE=-1.81D-09 OVMax= 9.10D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 4.77D-08 CP: 9.99D-01 1.09D+00 8.15D-01 9.24D-01 1.05D+00

CP: 1.18D+00 1.45D+00 9.44D-01 8.93D-01 8.30D-01

E= -1658.67658116344 Delta-E= -0.000000000283 Rises=F Damp=F

DIIS: error= 1.44D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67658116344 IErMin=11 ErrMin= 1.44D-07

ErrMax= 1.44D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.41D-11 BMatP= 8.88D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.113D-04 0.114D-03 0.371D-03 0.669D-03 0.180D-02-0.909D-03

Coeff-Com: -0.230D-01-0.203D-01 0.475D-02 0.210D+00 0.827D+00

Coeff: -0.113D-04 0.114D-03 0.371D-03 0.669D-03 0.180D-02-0.909D-03

Coeff: -0.230D-01-0.203D-01 0.475D-02 0.210D+00 0.827D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.15D-08 MaxDP=1.32D-06 DE=-2.83D-10 OVMax= 2.80D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.67D-08 CP: 9.99D-01 1.09D+00 8.15D-01 9.23D-01 1.05D+00

CP: 1.18D+00 1.45D+00 9.60D-01 9.31D-01 9.98D-01

CP: 1.03D+00

E= -1658.67658116346 Delta-E= -0.000000000017 Rises=F Damp=F

DIIS: error= 6.99D-08 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.67658116346 IErMin=12 ErrMin= 6.99D-08

ErrMax= 6.99D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.11D-11 BMatP= 7.41D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.368D-05-0.101D-03 0.818D-04 0.493D-03 0.216D-02 0.455D-02

Coeff-Com: -0.444D-02-0.234D-01-0.544D-01-0.107D-01 0.301D+00 0.785D+00

Coeff: 0.368D-05-0.101D-03 0.818D-04 0.493D-03 0.216D-02 0.455D-02

Coeff: -0.444D-02-0.234D-01-0.544D-01-0.107D-01 0.301D+00 0.785D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.27D-08 MaxDP=5.67D-07 DE=-1.68D-11 OVMax= 1.85D-06

Cycle 13 Pass 1 IDiag 1:

RMSU= 7.09D-09 CP: 9.99D-01 1.09D+00 8.15D-01 9.23D-01 1.05D+00

CP: 1.18D+00 1.45D+00 9.63D-01 9.40D-01 1.05D+00

CP: 1.19D+00 1.03D+00

E= -1658.67658116347 Delta-E= -0.000000000010 Rises=F Damp=F

DIIS: error= 2.99D-08 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1658.67658116347 IErMin=13 ErrMin= 2.99D-08

ErrMax= 2.99D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.21D-12 BMatP= 1.11D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.338D-05-0.606D-04-0.160D-04 0.114D-03 0.658D-03 0.211D-02

Coeff-Com: 0.222D-02-0.620D-02-0.256D-01-0.405D-01-0.177D-01 0.333D+00

Coeff-Com: 0.752D+00

Coeff: 0.338D-05-0.606D-04-0.160D-04 0.114D-03 0.658D-03 0.211D-02

Coeff: 0.222D-02-0.620D-02-0.256D-01-0.405D-01-0.177D-01 0.333D+00

Coeff: 0.752D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.37D-09 MaxDP=2.16D-07 DE=-1.05D-11 OVMax= 5.38D-07

Error on total polarization charges = 0.04168

SCF Done: E(UB3LYP) = -1658.67658116 A.U. after 13 cycles

NFock= 13 Conv=0.54D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655204995477D+03 PE=-6.145762599046D+03 EE= 1.730370842590D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.54

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:55:05 2019, MaxMem= 1342177280 cpu: 323.9

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 332

Leave Link 701 at Sat Aug 17 17:55:06 2019, MaxMem= 1342177280 cpu: 10.3

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:55:06 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:55:10 2019, MaxMem= 1342177280 cpu: 38.2

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.38376107D+00-2.87883640D+00 5.77016163D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000890817 -0.001978667 -0.006462598

2 6 -0.001527397 0.000965845 0.002027328

3 8 0.001385258 0.000345296 0.002229909

4 8 -0.000441089 0.000069118 0.000685681

5 6 0.001281950 -0.000913554 0.000738861

6 16 0.001853801 -0.000214804 -0.000598188

7 6 -0.001383642 -0.001202777 0.000517572

8 16 -0.001660115 0.000304483 -0.000049148

9 16 -0.000157204 0.000476146 -0.000570542

10 6 0.000291511 0.001208398 0.000580258

11 6 0.001023157 -0.000012957 -0.000318966

12 6 -0.000778322 -0.000147822 -0.001213540

13 6 -0.000508517 0.000515964 0.000511345

14 1 -0.000518604 -0.001236193 0.001385224

15 1 0.001436351 0.001710625 0.000880309

16 1 -0.000322786 0.000008763 0.000002236

17 1 0.000352054 0.000092865 -0.000132740

18 1 -0.000621253 0.001486712 0.000255075

19 1 0.001440262 -0.000364741 0.000219947

20 1 -0.000731094 -0.000846623 -0.000545282

21 1 -0.000133739 0.000477956 -0.000678401

22 1 0.000349451 -0.000080141 0.000353932

23 1 0.000108057 0.000117528 0.000603567

24 1 -0.000304611 -0.000747244 -0.000330484

25 1 -0.000164789 -0.000674796 0.000060769

26 1 0.000449583 0.000194266 -0.000331397

27 1 0.000172543 0.000446355 0.000179271

-------------------------------------------------------------------

Cartesian Forces: Max 0.006462598 RMS 0.001115417

Leave Link 716 at Sat Aug 17 17:55:10 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.002959708 RMS 0.000831708

Search for a local minimum.

Step number 54 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .83171D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43 45 44 47 46

49 48 51 50 53

54 52

ITU= 0 0 0 0 0 0 0 0 0 0 1 1 1 1 1 -1 -1 0 -1 -1

ITU= -1 0 -1 0 0 -1 -1 0 0 -1 0 0 -1 1 -1 1 -1 1 1 -1

ITU= 1 -1 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.99632.

Iteration 1 RMS(Cart)= 0.06732985 RMS(Int)= 0.00155420

Iteration 2 RMS(Cart)= 0.00350427 RMS(Int)= 0.00000215

Iteration 3 RMS(Cart)= 0.00000741 RMS(Int)= 0.00000027

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000027

ITry= 1 IFail=0 DXMaxC= 2.03D-01 DCOld= 1.00D+10 DXMaxT= 1.20D-01 DXLimC= 3.00D+00 Rises=T

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83774 -0.00015 -0.00202 0.00000 -0.00202 2.83572

R2 2.29002 -0.00167 -0.00070 0.00000 -0.00070 2.28931

R3 2.55789 -0.00186 -0.00471 0.00000 -0.00471 2.55318

R4 2.86728 0.00038 -0.00219 0.00000 -0.00219 2.86509

R5 3.58357 0.00104 0.02700 0.00000 0.02700 3.61056

R6 2.06002 -0.00066 -0.00194 0.00000 -0.00194 2.05808

R7 1.84034 -0.00200 -0.00339 0.00000 -0.00339 1.83694

R8 2.06200 -0.00025 -0.00075 0.00000 -0.00075 2.06124

R9 2.06965 -0.00034 -0.00102 0.00000 -0.00102 2.06863

R10 2.06484 -0.00162 -0.00477 0.00000 -0.00477 2.06007

R11 3.33512 -0.00222 -0.01989 0.00000 -0.01989 3.31523

R12 3.38959 -0.00062 -0.00193 0.00000 -0.00193 3.38766

R13 3.25331 0.00008 0.00054 0.00000 0.00054 3.25386

R14 3.47088 0.00111 0.00141 0.00000 0.00141 3.47228

R15 2.88048 0.00017 0.00089 0.00000 0.00089 2.88136

R16 2.06562 -0.00044 -0.00135 0.00000 -0.00135 2.06426

R17 2.06366 -0.00102 -0.00357 0.00000 -0.00357 2.06009

R18 2.89741 -0.00104 -0.00327 0.00000 -0.00327 2.89414

R19 2.07466 -0.00081 -0.00245 0.00000 -0.00245 2.07221

R20 2.07195 -0.00028 -0.00081 0.00000 -0.00081 2.07114

R21 2.88871 -0.00036 -0.00248 0.00000 -0.00248 2.88623

R22 2.07340 -0.00042 -0.00149 0.00000 -0.00149 2.07192

R23 2.07353 -0.00075 -0.00173 0.00000 -0.00173 2.07180

R24 2.06888 -0.00048 -0.00123 0.00000 -0.00123 2.06765

R25 2.07019 -0.00034 -0.00096 0.00000 -0.00096 2.06923

R26 2.07005 -0.00044 -0.00098 0.00000 -0.00098 2.06907

A1 2.18683 -0.00193 -0.01052 0.00000 -0.01052 2.17631

A2 1.97148 0.00035 0.00600 0.00000 0.00600 1.97748

A3 2.12356 0.00164 0.00526 0.00000 0.00526 2.12882

A4 2.00688 0.00281 0.02052 0.00000 0.02052 2.02740

A5 1.86226 -0.00296 -0.03310 0.00000 -0.03311 1.82915

A6 1.87145 -0.00022 0.00233 0.00000 0.00233 1.87379

A7 1.94764 0.00054 -0.00094 0.00000 -0.00094 1.94670

A8 1.94903 -0.00176 -0.00778 0.00000 -0.00778 1.94125

A9 1.81399 0.00138 0.01805 0.00000 0.01805 1.83203

A10 1.88414 -0.00239 -0.01177 0.00000 -0.01177 1.87237

A11 1.91390 -0.00002 -0.00097 0.00000 -0.00097 1.91293

A12 1.92854 0.00011 -0.00216 0.00000 -0.00216 1.92638

A13 1.95266 -0.00040 -0.00027 0.00000 -0.00027 1.95239

A14 1.88501 -0.00012 -0.00155 0.00000 -0.00155 1.88346

A15 1.89076 0.00031 0.00350 0.00000 0.00350 1.89426

A16 1.89129 0.00013 0.00151 0.00000 0.00151 1.89281

A17 1.78592 0.00067 0.01283 0.00000 0.01283 1.79875

A18 1.97433 -0.00106 -0.00416 0.00000 -0.00416 1.97016

A19 2.13856 -0.00016 0.00435 0.00000 0.00435 2.14291

A20 2.14536 0.00148 0.00973 0.00000 0.00973 2.15509

A21 1.78734 0.00099 0.00818 0.00000 0.00818 1.79552

A22 1.91993 0.00110 0.00655 0.00000 0.00655 1.92649

A23 1.86597 0.00091 0.01312 0.00000 0.01312 1.87908

A24 1.90442 -0.00116 -0.01227 0.00000 -0.01227 1.89215

A25 1.95009 -0.00166 -0.01077 0.00000 -0.01077 1.93932

A26 1.93622 0.00042 0.00191 0.00000 0.00191 1.93813

A27 1.88523 0.00038 0.00157 0.00000 0.00157 1.88680

A28 1.96065 -0.00093 -0.00764 0.00000 -0.00764 1.95301

A29 1.91581 0.00009 0.00023 0.00000 0.00023 1.91604

A30 1.91123 0.00062 0.00583 0.00000 0.00583 1.91706

A31 1.90647 0.00033 0.00048 0.00000 0.00048 1.90695

A32 1.90585 0.00015 0.00259 0.00000 0.00259 1.90844

A33 1.86113 -0.00022 -0.00116 0.00000 -0.00116 1.85997

A34 1.96277 0.00044 0.00326 0.00000 0.00326 1.96604

A35 1.90121 0.00014 0.00491 0.00000 0.00491 1.90612

A36 1.91490 -0.00049 -0.00700 0.00000 -0.00700 1.90790

A37 1.90935 -0.00005 0.00346 0.00000 0.00346 1.91280

A38 1.91641 -0.00012 -0.00356 0.00000 -0.00356 1.91285

A39 1.85607 0.00005 -0.00128 0.00000 -0.00128 1.85480

A40 1.94201 0.00060 0.00350 0.00000 0.00350 1.94551

A41 1.93926 0.00044 0.00284 0.00000 0.00284 1.94210

A42 1.94171 -0.00015 0.00111 0.00000 0.00111 1.94283

A43 1.88058 -0.00057 -0.00364 0.00000 -0.00364 1.87694

A44 1.88086 -0.00032 -0.00373 0.00000 -0.00373 1.87713

A45 1.87650 -0.00005 -0.00056 0.00000 -0.00056 1.87594

D1 2.64579 -0.00092 0.07163 0.00000 0.07162 2.71741

D2 -1.46779 -0.00058 0.05862 0.00000 0.05862 -1.40917

D3 0.46724 -0.00043 0.06534 0.00000 0.06534 0.53258

D4 -0.55047 0.00035 0.09026 0.00000 0.09026 -0.46021

D5 1.61914 0.00069 0.07725 0.00000 0.07725 1.69639

D6 -2.72902 0.00085 0.08398 0.00000 0.08398 -2.64504

D7 -3.09270 -0.00068 -0.00759 0.00000 -0.00759 -3.10030

D8 -0.00353 0.00042 0.00990 0.00000 0.00990 0.00637

D9 -3.09480 -0.00060 -0.04916 0.00000 -0.04916 3.13923

D10 -1.01887 -0.00069 -0.05299 0.00000 -0.05299 -1.07185

D11 1.09009 -0.00072 -0.05273 0.00000 -0.05273 1.03735

D12 1.06444 0.00081 -0.01948 0.00000 -0.01948 1.04496

D13 3.14037 0.00072 -0.02331 0.00000 -0.02331 3.11706

D14 -1.03386 0.00069 -0.02306 0.00000 -0.02306 -1.05692

D15 -0.95743 -0.00015 -0.03647 0.00000 -0.03647 -0.99390

D16 1.11851 -0.00024 -0.04030 0.00000 -0.04030 1.07821

D17 -3.05573 -0.00027 -0.04004 0.00000 -0.04004 -3.09577

D18 3.12900 -0.00106 0.06635 0.00000 0.06635 -3.08784

D19 -0.94862 0.00074 0.06830 0.00000 0.06830 -0.88032

D20 1.15432 -0.00024 0.06948 0.00000 0.06948 1.22380

D21 1.84501 0.00048 -0.02222 0.00000 -0.02222 1.82279

D22 -1.06468 -0.00089 -0.07451 0.00000 -0.07451 -1.13919

D23 2.53646 -0.00036 0.05599 0.00000 0.05599 2.59244

D24 -0.83808 0.00077 0.10786 0.00000 0.10786 -0.73021

D25 -3.01154 0.00046 -0.01907 0.00000 -0.01907 -3.03061

D26 -0.89092 -0.00036 -0.02017 0.00000 -0.02017 -0.91108

D27 1.14384 -0.00002 -0.01765 0.00000 -0.01765 1.12619

D28 -3.13126 0.00051 0.00683 0.00000 0.00683 -3.12444

D29 -1.00645 0.00037 0.00246 0.00000 0.00246 -1.00400

D30 1.03113 0.00051 0.00458 0.00000 0.00458 1.03572

D31 1.08232 -0.00029 -0.00697 0.00000 -0.00697 1.07536

D32 -3.07606 -0.00043 -0.01133 0.00000 -0.01134 -3.08739

D33 -1.03847 -0.00029 -0.00921 0.00000 -0.00921 -1.04768

D34 -1.02247 0.00007 -0.00298 0.00000 -0.00298 -1.02545

D35 1.10234 -0.00007 -0.00735 0.00000 -0.00735 1.09499

D36 3.13992 0.00007 -0.00522 0.00000 -0.00522 3.13470

D37 -3.11893 -0.00034 -0.01349 0.00000 -0.01349 -3.13242

D38 -0.99929 -0.00001 -0.00348 0.00000 -0.00348 -1.00277

D39 1.02594 -0.00014 -0.00615 0.00000 -0.00615 1.01979

D40 1.03413 -0.00006 -0.00904 0.00000 -0.00904 1.02509

D41 -3.12941 0.00027 0.00097 0.00000 0.00097 -3.12844

D42 -1.10418 0.00014 -0.00170 0.00000 -0.00170 -1.10588

D43 -0.99507 -0.00007 -0.00937 0.00000 -0.00937 -1.00444

D44 1.12457 0.00026 0.00064 0.00000 0.00064 1.12521

D45 -3.13338 0.00013 -0.00203 0.00000 -0.00203 -3.13541

D46 3.13742 0.00026 -0.00078 0.00000 -0.00078 3.13664

D47 -1.05026 0.00024 -0.00112 0.00000 -0.00112 -1.05137

D48 1.03989 0.00037 0.00083 0.00000 0.00083 1.04072

D49 1.02242 -0.00018 -0.01166 0.00000 -0.01166 1.01076

D50 3.11793 -0.00020 -0.01199 0.00000 -0.01199 3.10594

D51 -1.07510 -0.00007 -0.01004 0.00000 -0.01004 -1.08515

D52 -1.00831 -0.00014 -0.01007 0.00000 -0.01007 -1.01838

D53 1.08720 -0.00017 -0.01040 0.00000 -0.01040 1.07680

D54 -3.10583 -0.00004 -0.00845 0.00000 -0.00845 -3.11429

Item Value Threshold Converged?

Maximum Force 0.002960 0.000450 NO

RMS Force 0.000832 0.000300 NO

Maximum Displacement 0.202918 0.001800 NO

RMS Displacement 0.067857 0.001200 NO

Predicted change in Energy=-8.242947D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:55:10 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.094925 -0.405845 -0.206120

2 6 0 -2.844895 0.073820 0.471484

3 8 0 -4.888033 0.310229 -0.776939

4 8 0 -4.245141 -1.747848 -0.162580

5 6 0 -2.300140 -0.812537 1.574341

6 16 0 -1.577728 0.294506 -0.941344

7 6 0 -0.116133 0.765475 -0.093020

8 16 0 1.083031 -0.562305 0.019589

9 16 0 0.021925 2.246131 0.774979

10 6 0 2.687801 0.332393 -0.001741

11 6 0 3.846246 -0.656616 -0.070535

12 6 0 5.203726 0.052439 -0.065734

13 6 0 6.376667 -0.922406 -0.147116

14 1 0 -3.038847 1.081827 0.835371

15 1 0 -5.054846 -1.963880 -0.655150

16 1 0 -1.395012 -0.366649 1.988697

17 1 0 -3.030727 -0.905768 2.384189

18 1 0 -2.059046 -1.811486 1.210499

19 1 0 2.685452 0.996637 -0.868937

20 1 0 2.751012 0.947559 0.896037

21 1 0 3.795777 -1.347025 0.779904

22 1 0 3.759537 -1.268687 -0.975557

23 1 0 5.248166 0.752375 -0.908486

24 1 0 5.292507 0.659560 0.842840

25 1 0 7.335766 -0.395815 -0.147400

26 1 0 6.379372 -1.612579 0.702977

27 1 0 6.330645 -1.525142 -1.060026

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.500600 0.000000

3 O 1.211452 2.406005 0.000000

4 O 1.351086 2.383526 2.241970 0.000000

5 C 2.560604 1.516140 3.672371 2.770330 0.000000

6 S 2.714282 1.910628 3.314423 3.448590 2.841847

7 C 4.149164 2.871096 4.842109 4.834287 3.168612

8 S 5.185234 4.004680 6.086820 5.461511 3.731717

9 S 4.994395 3.609668 5.501259 5.919352 3.922552

10 C 6.825843 5.558914 7.615424 7.240094 5.354853

11 C 7.946286 6.752681 8.815976 8.165158 6.364589

12 C 9.310996 8.066558 10.120073 9.619329 7.729556

13 C 10.484490 9.295823 11.349428 10.653843 8.846607

14 H 2.100755 1.089087 2.571847 3.233900 2.163419

15 H 1.884290 3.210203 2.283468 0.972069 3.726208

16 H 3.479696 2.144320 4.506451 3.828699 1.090763

17 H 2.844669 2.156981 3.862766 2.944475 1.094670

18 H 2.850866 2.172114 4.056446 2.582326 1.090140

19 H 6.955559 5.764812 7.605084 7.487607 5.839422

20 H 7.064935 5.679599 7.846021 7.571793 5.391862

21 H 8.007574 6.797974 8.976570 8.105880 6.170658

22 H 7.939087 6.893096 8.792775 8.060111 6.590124

23 H 9.440770 8.237863 10.146690 9.845322 8.098783

24 H 9.505749 8.166903 10.314509 9.888033 7.768555

25 H 11.430846 10.210261 12.260346 11.659572 9.797384

26 H 10.582701 9.380012 11.525700 10.660570 8.759753

27 H 10.520194 9.438895 11.371344 10.616132 9.051969

6 7 8 9 10

6 S 0.000000

7 C 1.754344 0.000000

8 S 2.955868 1.792673 0.000000

9 S 3.051801 1.721867 3.095783 0.000000

10 C 4.367954 2.838651 1.837452 3.372326 0.000000

11 C 5.575163 4.209905 2.766293 4.875066 1.524751

12 C 6.842032 5.367501 4.167172 5.689477 2.532261

13 C 8.086041 6.708824 5.308488 7.160491 3.899151

14 H 2.431350 3.082896 4.512045 3.275298 5.835830

15 H 4.156027 5.670648 6.331920 6.748560 8.102370

16 H 3.009260 2.692727 3.171176 3.210520 4.595635

17 H 3.822438 4.174263 4.757341 4.673618 6.318803

18 H 3.049147 3.480632 3.584880 4.580870 5.347738

19 H 4.321219 2.916224 2.405730 3.370174 1.092361

20 H 4.747677 3.038406 2.414542 3.024709 1.090152

21 H 5.876383 4.530750 2.924527 5.210830 2.158477

22 H 5.561577 4.465143 2.941594 5.421076 2.158794

23 H 6.841312 5.425943 4.465205 5.690251 2.748461

24 H 7.107510 5.490031 4.459864 5.504620 2.757689

25 H 8.975370 7.542039 6.257180 7.830896 4.706918

26 H 8.346029 6.962782 5.442548 7.437201 4.231694

27 H 8.115883 6.909629 5.443352 7.575598 4.223827

11 12 13 14 15

11 C 0.000000

12 C 1.531513 0.000000

13 C 2.545493 1.527329 0.000000

14 H 7.158727 8.355337 9.676473 0.000000

15 H 9.015551 10.471449 11.490093 3.944900 0.000000

16 H 5.638732 6.923847 8.078957 2.475972 4.789098

17 H 7.306196 8.644449 9.742013 2.519809 3.801873

18 H 6.152012 7.605974 8.590391 3.077660 3.532519

19 H 2.172127 2.806839 4.222418 5.973235 8.289909

20 H 2.169603 2.782454 4.210737 5.791734 8.474319

21 H 1.096566 2.157758 2.775005 7.253585 8.987404

22 H 1.095999 2.158433 2.766874 7.417709 8.847559

23 H 2.157034 1.096411 2.158261 8.474914 10.658061

24 H 2.158296 1.096351 2.158248 8.342052 10.779337

25 H 3.500096 2.180182 1.094153 10.525297 12.499756

26 H 2.815832 2.178381 1.094990 9.796949 11.519951

27 H 2.811702 2.178835 1.094904 9.908391 11.401133

16 17 18 19 20

16 H 0.000000

17 H 1.767096 0.000000

18 H 1.770335 1.772579 0.000000

19 H 5.164765 6.846654 5.892357 0.000000

20 H 4.484480 6.251233 5.554086 1.766873 0.000000

21 H 5.419097 7.026350 5.888981 3.073149 2.523912

22 H 6.014137 7.584674 6.239341 2.509326 3.071113

23 H 7.333327 9.062627 8.028625 2.574631 3.087098

24 H 6.862142 8.608264 7.764442 3.136962 2.558313

25 H 8.988339 10.683312 9.597422 4.907643 4.890131

26 H 7.977873 9.585197 8.456006 4.787897 4.444836

27 H 8.385857 9.994075 8.696217 4.436588 4.770137

21 22 23 24 25

21 H 0.000000

22 H 1.757582 0.000000

23 H 3.060649 2.511017 0.000000

24 H 2.504105 3.061813 1.754345 0.000000

25 H 3.781033 3.773217 2.501133 2.503857 0.000000

26 H 2.598345 3.130379 3.077247 2.522588 1.765883

27 H 3.137295 2.585247 2.526224 3.077589 1.765937

26 27

26 H 0.000000

27 H 1.765843 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 3.85D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.104118 -0.463589 -0.130550

2 6 0 -2.848673 0.119438 0.448877

3 8 0 -4.901359 0.149553 -0.805888

4 8 0 -4.254517 -1.779661 0.135471

5 6 0 -2.295710 -0.573244 1.678960

6 16 0 -1.592437 0.101326 -0.990582

7 6 0 -0.124109 0.703654 -0.242961

8 16 0 1.075373 -0.589225 0.078568

9 16 0 0.021270 2.307233 0.367141

10 6 0 2.680280 0.286944 -0.102629

11 6 0 3.837768 -0.701760 -0.015715

12 6 0 5.195521 -0.003944 -0.138560

13 6 0 6.367412 -0.980784 -0.066514

14 1 0 -3.039396 1.174066 0.642513

15 1 0 -5.068111 -2.072821 -0.308421

16 1 0 -1.387214 -0.066486 2.006979

17 1 0 -3.020017 -0.530044 2.498604

18 1 0 -2.057842 -1.619009 1.483513

19 1 0 2.671452 0.798636 -1.067691

20 1 0 2.750707 1.042000 0.680545

21 1 0 3.793639 -1.241939 0.937551

22 1 0 3.743788 -1.454922 -0.806366

23 1 0 5.233684 0.546913 -1.085776

24 1 0 5.291598 0.744921 0.656397

25 1 0 7.326687 -0.463094 -0.161171

26 1 0 6.376454 -1.520876 0.885968

27 1 0 6.314061 -1.726112 -0.866798

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3048426 0.1933865 0.1808779

Leave Link 202 at Sat Aug 17 17:55:10 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.3206522212 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0549993219 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.2656528994 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2319

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.19D-11

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 95

GePol: Fraction of low-weight points (<1% of avg) = 4.10%

GePol: Cavity surface area = 309.197 Ang\*\*2

GePol: Cavity volume = 320.395 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057843440 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.2598685553 Hartrees.

Leave Link 301 at Sat Aug 17 17:55:10 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:55:10 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:55:10 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Lowest energy guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000031 0.000003 -0.000004 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999959 -0.008927 -0.000865 0.001081 Ang= -1.04 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 3.68D-03

Max alpha theta= 2.640 degrees.

Max beta theta= 2.139 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 17:55:11 2019, MaxMem= 1342177280 cpu: 4.3

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16133283.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.55D-15 for 2306.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.26D-15 for 672 463.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.22D-15 for 2301.

Iteration 1 A^-1\*A deviation from orthogonality is 1.10D-09 for 912 739.

Iteration 2 A\*A^-1 deviation from unit magnitude is 3.44D-15 for 259.

Iteration 2 A\*A^-1 deviation from orthogonality is 2.60D-15 for 2283 19.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 2203.

Iteration 2 A^-1\*A deviation from orthogonality is 4.84D-16 for 2291 1044.

E= -1658.67701756191

DIIS: error= 7.55D-07 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67701756191 IErMin= 1 ErrMin= 7.55D-07

ErrMax= 7.55D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.05D-09 BMatP= 1.05D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 88.590 Goal= None Shift= 0.000

Gap= 88.590 Goal= None Shift= 0.000

RMSDP=9.58D-08 MaxDP=2.34D-06 OVMax= 5.17D-06

Cycle 2 Pass 1 IDiag 1:

RMSU= 9.57D-08 CP: 1.00D+00

E= -1658.67701756222 Delta-E= -0.000000000312 Rises=F Damp=F

DIIS: error= 5.13D-07 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67701756222 IErMin= 2 ErrMin= 5.13D-07

ErrMax= 5.13D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.23D-10 BMatP= 1.05D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.278D+00 0.722D+00

Coeff: 0.278D+00 0.722D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.35D-08 MaxDP=2.12D-06 DE=-3.12D-10 OVMax= 3.76D-06

Cycle 3 Pass 1 IDiag 1:

RMSU= 4.28D-08 CP: 1.00D+00 9.22D-01

E= -1658.67701756222 Delta-E= -0.000000000006 Rises=F Damp=F

DIIS: error= 5.02D-07 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67701756222 IErMin= 3 ErrMin= 5.02D-07

ErrMax= 5.02D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.57D-10 BMatP= 3.23D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.225D-01 0.519D+00 0.504D+00

Coeff: -0.225D-01 0.519D+00 0.504D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.37D-08 MaxDP=1.04D-06 DE=-5.91D-12 OVMax= 2.06D-06

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.06D-08 CP: 1.00D+00 1.00D+00 5.39D-01

E= -1658.67701756232 Delta-E= -0.000000000097 Rises=F Damp=F

DIIS: error= 1.79D-07 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67701756232 IErMin= 4 ErrMin= 1.79D-07

ErrMax= 1.79D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.50D-11 BMatP= 3.23D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.222D-01 0.290D+00 0.306D+00 0.426D+00

Coeff: -0.222D-01 0.290D+00 0.306D+00 0.426D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.73D-09 MaxDP=1.92D-07 DE=-9.73D-11 OVMax= 5.14D-07

Error on total polarization charges = 0.04162

SCF Done: E(UB3LYP) = -1658.67701756 A.U. after 4 cycles

NFock= 4 Conv=0.57D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655236011718D+03 PE=-6.147285625529D+03 EE= 1.731112727694D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.63

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:55:22 2019, MaxMem= 1342177280 cpu: 128.9

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 335

Leave Link 701 at Sat Aug 17 17:55:23 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:55:23 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:55:26 2019, MaxMem= 1342177280 cpu: 38.3

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.40708721D+00-2.94569245D+00 6.35755943D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000016439 -0.000018819 0.000010466

2 6 -0.000013169 -0.000073582 0.000009528

3 8 -0.000031259 0.000109661 0.000030368

4 8 0.000066037 -0.000027594 -0.000001107

5 6 -0.000032086 -0.000039514 0.000026229

6 16 0.000058761 0.000066235 0.000002946

7 6 -0.000036526 0.000022671 0.000021699

8 16 0.000004543 0.000013221 0.000006664

9 16 -0.000028053 -0.000046066 0.000057560

10 6 0.000031448 -0.000007285 0.000025127

11 6 -0.000006687 0.000005465 -0.000013089

12 6 -0.000003714 0.000008574 -0.000025711

13 6 0.000002453 0.000003807 -0.000006715

14 1 -0.000013663 0.000011997 0.000023834

15 1 -0.000004290 0.000048823 -0.000040797

16 1 0.000016832 -0.000035632 0.000004828

17 1 0.000009475 -0.000052223 -0.000008715

18 1 0.000006576 -0.000023023 -0.000046440

19 1 0.000031042 0.000030036 0.000022591

20 1 -0.000042001 -0.000030554 0.000034169

21 1 -0.000000432 -0.000010840 -0.000035357

22 1 0.000002468 0.000007510 -0.000033293

23 1 0.000006493 0.000036207 0.000016007

24 1 -0.000001518 -0.000021648 0.000018543

25 1 0.000000593 0.000008369 -0.000011517

26 1 -0.000002330 -0.000024252 -0.000044479

27 1 -0.000004554 0.000038457 -0.000043336

-------------------------------------------------------------------

Cartesian Forces: Max 0.000109661 RMS 0.000030957

Leave Link 716 at Sat Aug 17 17:55:26 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000106216 RMS 0.000022354

Search for a local minimum.

Step number 55 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .22354D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43 45 44 47 46

49 48 51 50 53

54 55

ITU= 0 0 0 0 0 0 0 0 0 0 0 1 1 1 1 1 -1 -1 0 -1

ITU= -1 -1 0 -1 0 0 -1 -1 0 0 -1 0 0 -1 1 -1 1 -1 1 1

ITU= -1 1 -1 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Eigenvalues --- -0.00202 0.00000 0.00006 0.00047 0.00205

Eigenvalues --- 0.00285 0.00381 0.00552 0.01063 0.01683

Eigenvalues --- 0.02111 0.03175 0.03510 0.03704 0.04077

Eigenvalues --- 0.04539 0.04787 0.04890 0.04927 0.05251

Eigenvalues --- 0.05442 0.05484 0.05648 0.06011 0.06207

Eigenvalues --- 0.07992 0.08324 0.09377 0.11059 0.11212

Eigenvalues --- 0.11885 0.13112 0.14235 0.15368 0.15740

Eigenvalues --- 0.15947 0.16178 0.16291 0.16608 0.17433

Eigenvalues --- 0.18842 0.19448 0.20332 0.21895 0.22083

Eigenvalues --- 0.22499 0.23624 0.25035 0.25474 0.26183

Eigenvalues --- 0.26676 0.28398 0.29192 0.29517 0.29672

Eigenvalues --- 0.29751 0.31459 0.33262 0.33511 0.33873

Eigenvalues --- 0.33906 0.33939 0.34004 0.34045 0.34083

Eigenvalues --- 0.34138 0.34202 0.34406 0.34765 0.35104

Eigenvalues --- 0.35872 0.38090 0.49063 0.53159 0.84897

Eigenvalue 1 is -2.02D-03 should be greater than 0.000000 Eigenvector:

D2 D5 D1 D4 D3

1 -0.38526 -0.36924 -0.36589 -0.34986 -0.33066

D6 D25 D27 D26 D22

1 -0.31463 -0.19558 -0.18935 -0.17458 -0.08453

Eigenvalue 2 is 4.64D-06 Eigenvector:

D42 D41 D45 D40 D44

1 -0.22946 -0.21421 -0.21144 -0.20756 -0.19619

D39 D54 D43 D51 D48

1 -0.19163 0.19141 -0.18953 0.17950 0.17702

Eigenvalue 3 is 5.78D-05 Eigenvector:

D23 D20 D18 D19 D21

1 -0.38065 0.35347 0.29981 0.28276 0.26305

D24 D27 D26 D25 D15

1 -0.22541 -0.21473 -0.18880 -0.18295 -0.13373

Use linear search instead of GDIIS.

RFO step: Lambda=-2.01645179D-03 EMin=-2.01525075D-03

I= 1 Eig= -2.02D-03 Dot1= 1.47D-05

I= 1 Stepn= 2.99D-01 RXN= 2.99D-01 EDone=F

Mixed 1 eigenvectors in step. Raw Step.Grad= 1.47D-05.

RFO eigenvector is Hessian eigenvector with negative curvature.

Taking step of 2.99D-01 in eigenvector direction(s). Step.Grad= 5.55D-06.

Quartic linear search produced a step of -0.00129.

Iteration 1 RMS(Cart)= 0.06877978 RMS(Int)= 0.00295108

Iteration 2 RMS(Cart)= 0.00365293 RMS(Int)= 0.00002291

Iteration 3 RMS(Cart)= 0.00001445 RMS(Int)= 0.00002086

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00002086

ITry= 1 IFail=0 DXMaxC= 3.67D-01 DCOld= 1.00D+10 DXMaxT= 1.20D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83572 -0.00004 0.00000 0.01129 0.01129 2.84701

R2 2.28931 0.00006 0.00000 -0.00916 -0.00916 2.28015

R3 2.55318 0.00001 0.00001 -0.00098 -0.00097 2.55221

R4 2.86509 0.00001 0.00000 -0.00107 -0.00106 2.86402

R5 3.61056 0.00004 -0.00003 0.01820 0.01816 3.62873

R6 2.05808 0.00002 0.00000 0.00054 0.00054 2.05862

R7 1.83694 0.00000 0.00000 -0.00131 -0.00131 1.83564

R8 2.06124 0.00002 0.00000 0.00209 0.00209 2.06333

R9 2.06863 0.00000 0.00000 0.00046 0.00046 2.06908

R10 2.06007 0.00000 0.00001 -0.00082 -0.00081 2.05926

R11 3.31523 -0.00005 0.00003 -0.01500 -0.01497 3.30026

R12 3.38766 0.00003 0.00000 0.00570 0.00570 3.39336

R13 3.25386 -0.00003 0.00000 -0.00336 -0.00336 3.25050

R14 3.47228 0.00000 0.00000 0.00461 0.00461 3.47689

R15 2.88136 0.00000 0.00000 0.00035 0.00035 2.88172

R16 2.06426 0.00001 0.00000 0.00006 0.00006 2.06432

R17 2.06009 -0.00001 0.00000 -0.00142 -0.00142 2.05867

R18 2.89414 0.00001 0.00000 -0.00117 -0.00117 2.89297

R19 2.07221 -0.00001 0.00000 -0.00084 -0.00084 2.07137

R20 2.07114 0.00001 0.00000 0.00049 0.00049 2.07163

R21 2.88623 0.00000 0.00000 -0.00048 -0.00048 2.88575

R22 2.07192 0.00001 0.00000 -0.00091 -0.00091 2.07100

R23 2.07180 0.00000 0.00000 0.00045 0.00045 2.07225

R24 2.06765 0.00000 0.00000 -0.00010 -0.00010 2.06755

R25 2.06923 0.00000 0.00000 -0.00046 -0.00046 2.06877

R26 2.06907 0.00000 0.00000 0.00070 0.00070 2.06977

A1 2.17631 -0.00003 0.00001 -0.00054 -0.00053 2.17578

A2 1.97748 -0.00005 -0.00001 0.00314 0.00313 1.98061

A3 2.12882 0.00008 -0.00001 -0.00244 -0.00245 2.12637

A4 2.02740 0.00000 -0.00003 0.00327 0.00327 2.03067

A5 1.82915 0.00002 0.00004 0.01530 0.01537 1.84452

A6 1.87379 -0.00002 0.00000 -0.01588 -0.01593 1.85786

A7 1.94670 -0.00001 0.00000 -0.01524 -0.01524 1.93146

A8 1.94125 0.00001 0.00001 0.00009 0.00010 1.94134

A9 1.83203 0.00000 -0.00002 0.01430 0.01433 1.84636

A10 1.87237 -0.00004 0.00002 0.00768 0.00769 1.88007

A11 1.91293 -0.00001 0.00000 0.00157 0.00155 1.91449

A12 1.92638 0.00001 0.00000 0.00434 0.00435 1.93072

A13 1.95239 -0.00001 0.00000 -0.00841 -0.00842 1.94396

A14 1.88346 0.00000 0.00000 0.00173 0.00172 1.88518

A15 1.89426 0.00000 0.00000 -0.00604 -0.00607 1.88819

A16 1.89281 0.00001 0.00000 0.00702 0.00703 1.89983

A17 1.79875 -0.00011 -0.00002 -0.00433 -0.00435 1.79441

A18 1.97016 0.00000 0.00001 0.00492 0.00488 1.97505

A19 2.14291 -0.00004 -0.00001 -0.00006 -0.00011 2.14280

A20 2.15509 0.00003 -0.00001 -0.00197 -0.00203 2.15306

A21 1.79552 0.00008 -0.00001 0.01041 0.01040 1.80592

A22 1.92649 0.00002 -0.00001 0.00849 0.00848 1.93496

A23 1.87908 0.00002 -0.00002 0.00100 0.00096 1.88005

A24 1.89215 -0.00004 0.00002 -0.00944 -0.00942 1.88273

A25 1.93932 -0.00003 0.00001 0.00045 0.00045 1.93977

A26 1.93813 0.00003 0.00000 -0.00087 -0.00085 1.93727

A27 1.88680 0.00001 0.00000 -0.00001 -0.00001 1.88679

A28 1.95301 -0.00002 0.00001 -0.00246 -0.00245 1.95056

A29 1.91604 0.00000 0.00000 0.00140 0.00139 1.91744

A30 1.91706 0.00002 -0.00001 0.00652 0.00651 1.92357

A31 1.90695 0.00001 0.00000 -0.00197 -0.00197 1.90498

A32 1.90844 0.00000 0.00000 -0.00193 -0.00193 1.90651

A33 1.85997 -0.00001 0.00000 -0.00156 -0.00157 1.85840

A34 1.96604 0.00000 0.00000 0.00066 0.00066 1.96669

A35 1.90612 0.00001 -0.00001 0.00230 0.00229 1.90841

A36 1.90790 -0.00001 0.00001 -0.00298 -0.00297 1.90493

A37 1.91280 0.00000 0.00000 0.00034 0.00033 1.91314

A38 1.91285 0.00000 0.00000 -0.00054 -0.00053 1.91231

A39 1.85480 0.00000 0.00000 0.00018 0.00019 1.85498

A40 1.94551 0.00000 0.00000 0.00186 0.00186 1.94737

A41 1.94210 0.00001 0.00000 -0.00319 -0.00319 1.93891

A42 1.94283 -0.00001 0.00000 -0.00026 -0.00026 1.94256

A43 1.87694 0.00000 0.00000 0.00225 0.00225 1.87920

A44 1.87713 0.00000 0.00000 0.00076 0.00077 1.87790

A45 1.87594 0.00000 0.00000 -0.00133 -0.00134 1.87461

D1 2.71741 -0.00002 -0.00009 -0.10947 -0.10957 2.60785

D2 -1.40917 -0.00002 -0.00008 -0.11527 -0.11528 -1.52445

D3 0.53258 -0.00002 -0.00008 -0.09893 -0.09907 0.43350

D4 -0.46021 -0.00002 -0.00012 -0.10468 -0.10479 -0.56500

D5 1.69639 -0.00001 -0.00010 -0.11047 -0.11051 1.58588

D6 -2.64504 -0.00001 -0.00011 -0.09414 -0.09430 -2.73935

D7 -3.10030 0.00000 0.00001 0.00331 0.00332 -3.09698

D8 0.00637 0.00000 -0.00001 0.00800 0.00798 0.01435

D9 3.13923 0.00001 0.00006 0.00236 0.00243 -3.14153

D10 -1.07185 0.00001 0.00007 0.00810 0.00818 -1.06367

D11 1.03735 0.00002 0.00007 0.01435 0.01441 1.05176

D12 1.04496 -0.00001 0.00003 -0.00840 -0.00835 1.03661

D13 3.11706 -0.00001 0.00003 -0.00265 -0.00260 3.11446

D14 -1.05692 -0.00001 0.00003 0.00359 0.00363 -1.05329

D15 -0.99390 0.00000 0.00005 -0.01664 -0.01660 -1.01050

D16 1.07821 0.00000 0.00005 -0.01089 -0.01085 1.06736

D17 -3.09577 0.00000 0.00005 -0.00465 -0.00462 -3.10040

D18 -3.08784 0.00001 -0.00009 0.00076 0.00077 -3.08707

D19 -0.88032 0.00002 -0.00009 0.00586 0.00578 -0.87454

D20 1.22380 0.00002 -0.00009 0.00650 0.00630 1.23010

D21 1.82279 -0.00003 0.00003 -0.00833 -0.00830 1.81449

D22 -1.13919 0.00003 0.00010 -0.02529 -0.02520 -1.16439

D23 2.59244 0.00004 -0.00007 -0.00870 -0.00877 2.58367

D24 -0.73021 -0.00002 -0.00014 0.00863 0.00849 -0.72173

D25 -3.03061 0.00000 0.00002 -0.05852 -0.05851 -3.08912

D26 -0.91108 -0.00001 0.00003 -0.05223 -0.05220 -0.96329

D27 1.12619 -0.00002 0.00002 -0.05665 -0.05662 1.06958

D28 -3.12444 0.00001 -0.00001 -0.01300 -0.01301 -3.13744

D29 -1.00400 0.00001 0.00000 -0.01618 -0.01618 -1.02018

D30 1.03572 0.00001 -0.00001 -0.01343 -0.01343 1.02229

D31 1.07536 -0.00001 0.00001 -0.02009 -0.02008 1.05527

D32 -3.08739 -0.00001 0.00001 -0.02327 -0.02326 -3.11065

D33 -1.04768 -0.00001 0.00001 -0.02051 -0.02050 -1.06818

D34 -1.02545 -0.00001 0.00000 -0.01980 -0.01979 -1.04524

D35 1.09499 -0.00001 0.00001 -0.02298 -0.02297 1.07202

D36 3.13470 -0.00001 0.00001 -0.02023 -0.02022 3.11449

D37 -3.13242 -0.00001 0.00002 -0.01944 -0.01942 3.13134

D38 -1.00277 -0.00001 0.00000 -0.01692 -0.01692 -1.01969

D39 1.01979 -0.00001 0.00001 -0.01708 -0.01707 1.00272

D40 1.02509 0.00000 0.00001 -0.01822 -0.01821 1.00689

D41 -3.12844 0.00000 0.00000 -0.01570 -0.01570 3.13904

D42 -1.10588 0.00000 0.00000 -0.01586 -0.01586 -1.12174

D43 -1.00444 0.00000 0.00001 -0.01415 -0.01414 -1.01858

D44 1.12521 0.00000 0.00000 -0.01164 -0.01164 1.11357

D45 -3.13541 0.00001 0.00000 -0.01180 -0.01180 3.13598

D46 3.13664 0.00001 0.00000 -0.01639 -0.01638 3.12025

D47 -1.05137 0.00001 0.00000 -0.01443 -0.01444 -1.06581

D48 1.04072 0.00001 0.00000 -0.01844 -0.01844 1.02228

D49 1.01076 0.00000 0.00002 -0.02002 -0.02000 0.99077

D50 3.10594 0.00000 0.00002 -0.01806 -0.01805 3.08789

D51 -1.08515 0.00000 0.00001 -0.02207 -0.02206 -1.10721

D52 -1.01838 0.00000 0.00001 -0.02012 -0.02011 -1.03849

D53 1.07680 0.00000 0.00001 -0.01817 -0.01816 1.05864

D54 -3.11429 0.00000 0.00001 -0.02218 -0.02217 -3.13646

Item Value Threshold Converged?

Maximum Force 0.000106 0.000450 YES

RMS Force 0.000022 0.000300 YES

Maximum Displacement 0.366867 0.001800 NO

RMS Displacement 0.069243 0.001200 NO

Predicted change in Energy=-1.051919D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:55:27 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.124656 -0.388929 -0.157794

2 6 0 -2.848839 0.074791 0.495674

3 8 0 -4.983750 0.344025 -0.582801

4 8 0 -4.216083 -1.731983 -0.266847

5 6 0 -2.264162 -0.839373 1.553704

6 16 0 -1.598248 0.339703 -0.937213

7 6 0 -0.133410 0.782748 -0.095817

8 16 0 1.069336 -0.548628 -0.022689

9 16 0 0.026320 2.251249 0.785490

10 6 0 2.684965 0.331190 -0.052069

11 6 0 3.843226 -0.660541 -0.070358

12 6 0 5.198870 0.050456 -0.089061

13 6 0 6.374797 -0.923780 -0.093143

14 1 0 -3.051619 1.066147 0.899201

15 1 0 -5.044082 -1.935123 -0.732385

16 1 0 -1.347203 -0.401044 1.952741

17 1 0 -2.966944 -0.967915 2.383408

18 1 0 -2.021887 -1.818998 1.142475

19 1 0 2.699454 0.970253 -0.937906

20 1 0 2.733080 0.971394 0.828055

21 1 0 3.790509 -1.310966 0.810350

22 1 0 3.766983 -1.315839 -0.945890

23 1 0 5.256068 0.699850 -0.970012

24 1 0 5.271227 0.709809 0.784165

25 1 0 7.333287 -0.397362 -0.128261

26 1 0 6.371691 -1.548797 0.805644

27 1 0 6.333231 -1.593974 -0.958437

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.506574 0.000000

3 O 1.206605 2.406957 0.000000

4 O 1.350572 2.390655 2.235833 0.000000

5 C 2.567793 1.515576 3.655304 2.814455 0.000000

6 S 2.742469 1.920239 3.404005 3.405045 2.835195

7 C 4.160134 2.867859 4.894429 4.798056 3.145203

8 S 5.198202 4.001180 6.144136 5.421770 3.698886

9 S 5.009084 3.617665 5.532678 5.913673 3.922806

10 C 6.848407 5.566753 7.687069 7.206058 5.333159

11 C 7.972990 6.756096 8.898722 8.132593 6.322164

12 C 9.334127 8.068960 10.198810 9.583843 7.693330

13 C 10.513266 9.296198 11.439567 10.623093 8.794933

14 H 2.094252 1.089375 2.539866 3.247333 2.163208

15 H 1.888443 3.219780 2.284849 0.971378 3.762291

16 H 3.488373 2.145780 4.495395 3.863734 1.091868

17 H 2.851881 2.159797 3.819305 3.027870 1.094912

18 H 2.856122 2.165327 4.053132 2.609264 1.089712

19 H 7.001745 5.800048 7.716857 7.455002 5.841264

20 H 7.060519 5.663232 7.869789 7.536440 5.364502

21 H 8.027284 6.789719 9.037007 8.089693 6.118335

22 H 7.984875 6.912384 8.914164 8.022694 6.545969

23 H 9.478561 8.260051 10.253313 9.804586 8.080360

24 H 9.506689 8.149966 10.352147 9.852717 7.731381

25 H 11.457984 10.212145 12.347699 11.627053 9.753739

26 H 10.604094 9.367512 11.595542 10.643531 8.697174

27 H 10.557488 9.445084 11.487863 10.572860 8.988629

6 7 8 9 10

6 S 0.000000

7 C 1.746422 0.000000

8 S 2.956601 1.795691 0.000000

9 S 3.043178 1.720090 3.095214 0.000000

10 C 4.373724 2.854654 1.839892 3.384748 0.000000

11 C 5.600140 4.230528 2.776556 4.876451 1.524938

12 C 6.855935 5.382333 4.173292 5.688902 2.529803

13 C 8.116544 6.728224 5.319175 7.152340 3.897628

14 H 2.452024 3.096178 4.521022 3.300167 5.861182

15 H 4.134073 5.648606 6.308718 6.748232 8.083141

16 H 2.993921 2.659181 3.124703 3.206820 4.562215

17 H 3.822265 4.152143 4.717696 4.677177 6.289936

18 H 3.027303 3.445112 3.539365 4.570504 5.310810

19 H 4.343713 2.961316 2.408715 3.428803 1.092391

20 H 4.719704 3.017597 2.408792 2.994393 1.089401

21 H 5.900626 4.538933 2.946167 5.182578 2.159323

22 H 5.614855 4.509962 2.952662 5.451087 2.163882

23 H 6.863850 5.460546 4.470442 5.730523 2.754833

24 H 7.091531 5.476293 4.459884 5.466726 2.744338

25 H 8.998333 7.559449 6.266667 7.825717 4.705687

26 H 8.374002 6.968864 5.459070 7.396248 4.226343

27 H 8.163817 6.943368 5.447657 7.589739 4.223459

11 12 13 14 15

11 C 0.000000

12 C 1.530894 0.000000

13 C 2.545322 1.527074 0.000000

14 H 7.173589 8.371311 9.685136 0.000000

15 H 9.002616 10.453443 11.481387 3.954694 0.000000

16 H 5.576812 6.871964 8.005509 2.483470 4.819774

17 H 7.245265 8.592479 9.664542 2.519414 3.867578

18 H 6.100209 7.559820 8.534194 3.073043 3.558406

19 H 2.172636 2.795290 4.220087 6.038128 8.273198

20 H 2.168590 2.787355 4.207421 5.785912 8.447904

21 H 1.096120 2.155433 2.764915 7.243844 8.989973

22 H 1.096259 2.156668 2.771566 7.454632 8.835382

23 H 2.157815 1.095928 2.157922 8.523250 10.634503

24 H 2.155749 1.096588 2.157811 8.331265 10.756449

25 H 3.500449 2.181241 1.094099 10.537732 12.487151

26 H 2.819488 2.175688 1.094748 9.779849 11.525392

27 H 2.803587 2.178701 1.095273 9.929877 11.384671

16 17 18 19 20

16 H 0.000000

17 H 1.769287 0.000000

18 H 1.767010 1.776904 0.000000

19 H 5.158656 6.848043 5.865064 0.000000

20 H 4.449407 6.218546 5.522216 1.766281 0.000000

21 H 5.341264 6.946608 5.844002 3.074210 2.515480

22 H 5.949270 7.520044 6.174582 2.523073 3.073641

23 H 7.304632 9.035751 7.985978 2.571075 3.110024

24 H 6.811988 8.558025 7.727404 3.106023 2.551968

25 H 8.926449 10.617381 9.547518 4.898806 4.893867

26 H 7.887617 9.488776 8.404678 4.782354 4.426212

27 H 8.299826 9.902178 8.618147 4.447473 4.767992

21 22 23 24 25

21 H 0.000000

22 H 1.756405 0.000000

23 H 3.059565 2.506184 0.000000

24 H 2.505343 3.059262 1.754270 0.000000

25 H 3.777160 3.772352 2.495447 2.512058 0.000000

26 H 2.592120 3.147483 3.074733 2.512525 1.767102

27 H 3.110327 2.581306 2.534175 3.077650 1.766688

26 27

26 H 0.000000

27 H 1.765079 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 9.08D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.123385 -0.464347 -0.092444

2 6 0 -2.845408 0.106167 0.465281

3 8 0 -4.986676 0.183974 -0.631242

4 8 0 -4.211756 -1.806507 0.029390

5 6 0 -2.252715 -0.613363 1.660254

6 16 0 -1.603084 0.125318 -0.998817

7 6 0 -0.135046 0.707808 -0.253457

8 16 0 1.071658 -0.589525 0.038607

9 16 0 0.025345 2.305256 0.363909

10 6 0 2.684728 0.275281 -0.149319

11 6 0 3.845551 -0.703023 -0.004939

12 6 0 5.199153 -0.003212 -0.152122

13 6 0 6.377669 -0.961825 0.003180

14 1 0 -3.048742 1.151414 0.695178

15 1 0 -5.041638 -2.087446 -0.390066

16 1 0 -1.334859 -0.111845 1.973618

17 1 0 -2.950778 -0.599924 2.503676

18 1 0 -2.009959 -1.648294 1.420546

19 1 0 2.692837 0.754123 -1.131136

20 1 0 2.735738 1.056142 0.608604

21 1 0 3.799219 -1.194002 0.973976

22 1 0 3.766479 -1.498025 -0.755607

23 1 0 5.249968 0.486718 -1.131124

24 1 0 5.274317 0.795386 0.595606

25 1 0 7.334536 -0.447391 -0.126499

26 1 0 6.380973 -1.424600 0.995300

27 1 0 6.333367 -1.769700 -0.735060

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3143568 0.1929467 0.1800850

Leave Link 202 at Sat Aug 17 17:55:27 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1101.5472084509 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0549675553 Hartrees.

Nuclear repulsion after empirical dispersion term = 1101.4922408956 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2322

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.28D-08

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 99

GePol: Fraction of low-weight points (<1% of avg) = 4.26%

GePol: Cavity surface area = 309.775 Ang\*\*2

GePol: Cavity volume = 321.030 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057388495 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1101.4865020460 Hartrees.

Leave Link 301 at Sat Aug 17 17:55:27 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.86D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:55:27 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:55:27 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999988 -0.004737 -0.000968 -0.000687 Ang= -0.56 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.63011913718

Leave Link 401 at Sat Aug 17 17:55:28 2019, MaxMem= 1342177280 cpu: 7.7

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16175052.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.77D-15 for 2320.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.47D-15 for 829 402.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.77D-15 for 2314.

Iteration 1 A^-1\*A deviation from orthogonality is 2.73D-11 for 798 718.

E= -1658.65406341751

DIIS: error= 7.50D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.65406341751 IErMin= 1 ErrMin= 7.50D-03

ErrMax= 7.50D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.27D-02 BMatP= 5.27D-02

IDIUse=3 WtCom= 9.25D-01 WtEn= 7.50D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.429 Goal= None Shift= 0.000

Gap= 0.484 Goal= None Shift= 0.000

GapD= 0.429 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=4.58D-04 MaxDP=1.41D-02 OVMax= 3.49D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.58D-04 CP: 9.99D-01

E= -1658.67632459045 Delta-E= -0.022261172941 Rises=F Damp=F

DIIS: error= 9.69D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67632459045 IErMin= 2 ErrMin= 9.69D-04

ErrMax= 9.69D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.06D-03 BMatP= 5.27D-02

IDIUse=3 WtCom= 9.90D-01 WtEn= 9.69D-03

Coeff-Com: -0.631D-01 0.106D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.625D-01 0.106D+01

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=7.57D-05 MaxDP=2.44D-03 DE=-2.23D-02 OVMax= 6.14D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 6.92D-05 CP: 9.99D-01 1.07D+00

E= -1658.67649191032 Delta-E= -0.000167319871 Rises=F Damp=F

DIIS: error= 7.10D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67649191032 IErMin= 3 ErrMin= 7.10D-04

ErrMax= 7.10D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.96D-04 BMatP= 1.06D-03

IDIUse=3 WtCom= 9.93D-01 WtEn= 7.10D-03

Coeff-Com: -0.394D-01 0.522D+00 0.517D+00

Coeff-En: 0.000D+00 0.849D-01 0.915D+00

Coeff: -0.391D-01 0.519D+00 0.520D+00

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=5.07D-05 MaxDP=1.94D-03 DE=-1.67D-04 OVMax= 4.03D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 3.30D-05 CP: 9.99D-01 1.08D+00 4.51D-01

E= -1658.67660384378 Delta-E= -0.000111933457 Rises=F Damp=F

DIIS: error= 4.91D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67660384378 IErMin= 4 ErrMin= 4.91D-04

ErrMax= 4.91D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.24D-04 BMatP= 7.96D-04

IDIUse=3 WtCom= 9.95D-01 WtEn= 4.91D-03

Coeff-Com: -0.123D-01 0.153D+00 0.348D+00 0.511D+00

Coeff-En: 0.000D+00 0.000D+00 0.256D+00 0.744D+00

Coeff: -0.122D-01 0.153D+00 0.348D+00 0.512D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=2.12D-05 MaxDP=8.71D-04 DE=-1.12D-04 OVMax= 1.87D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 8.31D-06 CP: 9.99D-01 1.08D+00 6.58D-01 6.05D-01

E= -1658.67664697208 Delta-E= -0.000043128304 Rises=F Damp=F

DIIS: error= 1.27D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67664697208 IErMin= 5 ErrMin= 1.27D-04

ErrMax= 1.27D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.09D-05 BMatP= 2.24D-04

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.27D-03

Coeff-Com: -0.431D-02 0.512D-01 0.165D+00 0.289D+00 0.499D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.430D-02 0.511D-01 0.165D+00 0.288D+00 0.500D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=4.49D-06 MaxDP=2.07D-04 DE=-4.31D-05 OVMax= 3.96D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.93D-06 CP: 9.99D-01 1.08D+00 6.55D-01 6.63D-01 6.63D-01

E= -1658.67664901038 Delta-E= -0.000002038291 Rises=F Damp=F

DIIS: error= 3.06D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67664901038 IErMin= 6 ErrMin= 3.06D-05

ErrMax= 3.06D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.81D-07 BMatP= 1.09D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.611D-03-0.123D-01 0.263D-02 0.263D-01 0.235D+00 0.748D+00

Coeff: 0.611D-03-0.123D-01 0.263D-02 0.263D-01 0.235D+00 0.748D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=1.48D-06 MaxDP=7.02D-05 DE=-2.04D-06 OVMax= 1.36D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 9.87D-07 CP: 9.99D-01 1.08D+00 6.63D-01 6.78D-01 7.55D-01

CP: 9.45D-01

E= -1658.67664918018 Delta-E= -0.000000169799 Rises=F Damp=F

DIIS: error= 7.80D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67664918018 IErMin= 7 ErrMin= 7.80D-06

ErrMax= 7.80D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.63D-08 BMatP= 8.81D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.516D-03-0.892D-02-0.626D-02 0.636D-03 0.102D+00 0.386D+00

Coeff-Com: 0.526D+00

Coeff: 0.516D-03-0.892D-02-0.626D-02 0.636D-03 0.102D+00 0.386D+00

Coeff: 0.526D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=6.36D-07 MaxDP=2.71D-05 DE=-1.70D-07 OVMax= 7.32D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 5.04D-07 CP: 9.99D-01 1.08D+00 6.67D-01 6.75D-01 7.83D-01

CP: 9.99D-01 9.10D-01

E= -1658.67664919861 Delta-E= -0.000000018439 Rises=F Damp=F

DIIS: error= 3.60D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67664919861 IErMin= 8 ErrMin= 3.60D-06

ErrMax= 3.60D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.48D-08 BMatP= 8.63D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.131D-03-0.185D-02-0.343D-02-0.463D-02 0.563D-02 0.420D-01

Coeff-Com: 0.282D+00 0.680D+00

Coeff: 0.131D-03-0.185D-02-0.343D-02-0.463D-02 0.563D-02 0.420D-01

Coeff: 0.282D+00 0.680D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=3.24D-07 MaxDP=1.55D-05 DE=-1.84D-08 OVMax= 4.26D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.15D-07 CP: 9.99D-01 1.08D+00 6.67D-01 6.78D-01 7.87D-01

CP: 1.03D+00 1.09D+00 8.86D-01

E= -1658.67664920294 Delta-E= -0.000000004325 Rises=F Damp=F

DIIS: error= 1.42D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67664920294 IErMin= 9 ErrMin= 1.42D-06

ErrMax= 1.42D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.87D-09 BMatP= 1.48D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.351D-04 0.907D-03-0.666D-03-0.307D-02-0.188D-01-0.607D-01

Coeff-Com: 0.544D-01 0.434D+00 0.594D+00

Coeff: -0.351D-04 0.907D-03-0.666D-03-0.307D-02-0.188D-01-0.607D-01

Coeff: 0.544D-01 0.434D+00 0.594D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=2.15D-07 MaxDP=1.30D-05 DE=-4.33D-09 OVMax= 2.89D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 8.86D-08 CP: 9.99D-01 1.08D+00 6.68D-01 6.78D-01 7.92D-01

CP: 1.06D+00 1.19D+00 1.11D+00 8.51D-01

E= -1658.67664920447 Delta-E= -0.000000001529 Rises=F Damp=F

DIIS: error= 8.06D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67664920447 IErMin=10 ErrMin= 8.06D-07

ErrMax= 8.06D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.53D-10 BMatP= 4.87D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.403D-04 0.777D-03 0.304D-03-0.742D-03-0.102D-01-0.372D-01

Coeff-Com: -0.380D-01 0.663D-01 0.274D+00 0.745D+00

Coeff: -0.403D-04 0.777D-03 0.304D-03-0.742D-03-0.102D-01-0.372D-01

Coeff: -0.380D-01 0.663D-01 0.274D+00 0.745D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=8.72D-08 MaxDP=3.86D-06 DE=-1.53D-09 OVMax= 8.69D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 4.08D-08 CP: 9.99D-01 1.08D+00 6.68D-01 6.78D-01 7.95D-01

CP: 1.07D+00 1.24D+00 1.19D+00 9.87D-01 9.03D-01

E= -1658.67664920471 Delta-E= -0.000000000241 Rises=F Damp=F

DIIS: error= 3.22D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67664920471 IErMin=11 ErrMin= 3.22D-07

ErrMax= 3.22D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.31D-10 BMatP= 5.53D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.121D-04 0.163D-03 0.282D-03 0.312D-03-0.528D-03-0.380D-02

Coeff-Com: -0.314D-01-0.652D-01-0.747D-02 0.384D+00 0.724D+00

Coeff: -0.121D-04 0.163D-03 0.282D-03 0.312D-03-0.528D-03-0.380D-02

Coeff: -0.314D-01-0.652D-01-0.747D-02 0.384D+00 0.724D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=5.04D-08 MaxDP=2.58D-06 DE=-2.41D-10 OVMax= 7.61D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.82D-08 CP: 9.99D-01 1.08D+00 6.68D-01 6.78D-01 7.96D-01

CP: 1.08D+00 1.26D+00 1.23D+00 1.05D+00 1.15D+00

CP: 8.06D-01

E= -1658.67664920475 Delta-E= -0.000000000044 Rises=F Damp=F

DIIS: error= 1.03D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.67664920475 IErMin=12 ErrMin= 1.03D-07

ErrMax= 1.03D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.50D-11 BMatP= 1.31D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.169D-05-0.623D-04 0.732D-04 0.259D-03 0.152D-02 0.468D-02

Coeff-Com: -0.665D-02-0.380D-01-0.493D-01 0.296D-01 0.300D+00 0.758D+00

Coeff: 0.169D-05-0.623D-04 0.732D-04 0.259D-03 0.152D-02 0.468D-02

Coeff: -0.665D-02-0.380D-01-0.493D-01 0.296D-01 0.300D+00 0.758D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=1.33D-08 MaxDP=7.04D-07 DE=-4.37D-11 OVMax= 1.18D-06

Cycle 13 Pass 1 IDiag 1:

RMSU= 6.24D-09 CP: 9.99D-01 1.08D+00 6.68D-01 6.78D-01 7.96D-01

CP: 1.08D+00 1.26D+00 1.24D+00 1.07D+00 1.20D+00

CP: 9.72D-01 9.03D-01

E= -1658.67664920478 Delta-E= -0.000000000023 Rises=F Damp=F

DIIS: error= 3.14D-08 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1658.67664920478 IErMin=13 ErrMin= 3.14D-08

ErrMax= 3.14D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.07D-12 BMatP= 1.50D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.145D-05-0.303D-04 0.104D-05 0.542D-04 0.491D-03 0.159D-02

Coeff-Com: 0.920D-03-0.478D-02-0.136D-01-0.240D-01 0.254D-01 0.211D+00

Coeff-Com: 0.803D+00

Coeff: 0.145D-05-0.303D-04 0.104D-05 0.542D-04 0.491D-03 0.159D-02

Coeff: 0.920D-03-0.478D-02-0.136D-01-0.240D-01 0.254D-01 0.211D+00

Coeff: 0.803D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=4.26D-09 MaxDP=1.81D-07 DE=-2.32D-11 OVMax= 5.22D-07

Error on total polarization charges = 0.04162

SCF Done: E(UB3LYP) = -1658.67664920 A.U. after 13 cycles

NFock= 13 Conv=0.43D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655243676343D+03 PE=-6.145736332539D+03 EE= 1.730329504945D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.60

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:55:56 2019, MaxMem= 1342177280 cpu: 326.3

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 336

Leave Link 701 at Sat Aug 17 17:55:57 2019, MaxMem= 1342177280 cpu: 10.5

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:55:57 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:56:00 2019, MaxMem= 1342177280 cpu: 37.2

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.45489907D+00-2.97852458D+00 5.56399778D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.006149274 -0.003743537 0.002896151

2 6 -0.001753364 -0.000026691 -0.001459915

3 8 -0.004563025 0.005243339 -0.002913028

4 8 0.002374779 -0.001433884 0.001039912

5 6 0.000031920 -0.000523201 -0.000226199

6 16 -0.003969105 -0.000682232 0.000113684

7 6 0.003076548 0.000600062 0.000360065

8 16 0.000216086 -0.001024507 -0.000232382

9 16 0.000436344 0.000814272 0.000794154

10 6 -0.001343713 0.000605083 -0.000066295

11 6 -0.000342210 -0.000536298 -0.000259035

12 6 0.000211377 0.000587098 0.000366587

13 6 -0.000238820 -0.000755367 -0.000061125

14 1 0.001369388 0.000208908 -0.000630674

15 1 -0.000515473 0.000539186 0.000002940

16 1 -0.000940866 0.000045738 -0.000114841

17 1 0.000053406 -0.000232569 -0.000216193

18 1 -0.000381205 -0.000888773 0.000542451

19 1 0.000126182 0.000047918 -0.000065760

20 1 0.000427259 0.000373006 0.000320805

21 1 -0.000357182 -0.000064000 0.000182080

22 1 -0.000451955 0.000311819 -0.000102043

23 1 -0.000137816 0.000172625 -0.000220379

24 1 0.000218936 0.000021539 -0.000166386

25 1 -0.000043327 0.000012228 0.000148553

26 1 0.000279993 -0.000083988 0.000076146

27 1 0.000066571 0.000412226 -0.000109273

-------------------------------------------------------------------

Cartesian Forces: Max 0.006149274 RMS 0.001450646

Leave Link 716 at Sat Aug 17 17:56:00 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.007455040 RMS 0.001090366

Search for a local minimum.

Step number 56 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .10904D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43 45 44 47 46

49 48 51 50 53

54 56 52

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 1 1 1 1 1 -1 -1 0

ITU= -1 -1 -1 0 -1 0 0 -1 -1 0 0 -1 0 0 -1 1 -1 1 -1 1

ITU= 1 -1 1 -1 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.98039.

Iteration 1 RMS(Cart)= 0.06780241 RMS(Int)= 0.00284329

Iteration 2 RMS(Cart)= 0.00349448 RMS(Int)= 0.00000929

Iteration 3 RMS(Cart)= 0.00001400 RMS(Int)= 0.00000040

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000040

ITry= 1 IFail=0 DXMaxC= 3.60D-01 DCOld= 1.00D+10 DXMaxT= 1.20D-01 DXLimC= 3.00D+00 Rises=T

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.84701 -0.00355 -0.01108 0.00000 -0.01108 2.83594

R2 2.28015 0.00746 0.00898 0.00000 0.00898 2.28913

R3 2.55221 0.00071 0.00093 0.00000 0.00093 2.55315

R4 2.86402 0.00043 0.00104 0.00000 0.00104 2.86506

R5 3.62873 -0.00185 -0.01771 0.00000 -0.01771 3.61102

R6 2.05862 -0.00030 -0.00054 0.00000 -0.00054 2.05808

R7 1.83564 0.00031 0.00127 0.00000 0.00127 1.83691

R8 2.06333 -0.00080 -0.00205 0.00000 -0.00205 2.06128

R9 2.06908 -0.00017 -0.00045 0.00000 -0.00045 2.06863

R10 2.05926 0.00048 0.00078 0.00000 0.00078 2.06003

R11 3.30026 0.00261 0.01461 0.00000 0.01461 3.31486

R12 3.39336 -0.00093 -0.00560 0.00000 -0.00560 3.38777

R13 3.25050 0.00113 0.00329 0.00000 0.00329 3.25379

R14 3.47689 -0.00090 -0.00452 0.00000 -0.00452 3.47238

R15 2.88172 -0.00062 -0.00034 0.00000 -0.00034 2.88137

R16 2.06432 0.00009 -0.00006 0.00000 -0.00006 2.06426

R17 2.05867 0.00048 0.00138 0.00000 0.00138 2.06005

R18 2.89297 0.00047 0.00114 0.00000 0.00114 2.89411

R19 2.07137 0.00021 0.00082 0.00000 0.00082 2.07218

R20 2.07163 -0.00008 -0.00048 0.00000 -0.00048 2.07115

R21 2.88575 0.00033 0.00046 0.00000 0.00046 2.88622

R22 2.07100 0.00027 0.00089 0.00000 0.00089 2.07189

R23 2.07225 -0.00011 -0.00045 0.00000 -0.00045 2.07181

R24 2.06755 -0.00004 0.00009 0.00000 0.00009 2.06764

R25 2.06877 0.00013 0.00044 0.00000 0.00044 2.06922

R26 2.06977 -0.00018 -0.00069 0.00000 -0.00069 2.06908

A1 2.17578 0.00021 0.00048 0.00000 0.00048 2.17626

A2 1.98061 -0.00240 -0.00304 0.00000 -0.00304 1.97756

A3 2.12637 0.00218 0.00242 0.00000 0.00242 2.12879

A4 2.03067 -0.00225 -0.00313 0.00000 -0.00313 2.02754

A5 1.84452 -0.00117 -0.01519 0.00000 -0.01519 1.82933

A6 1.85786 0.00163 0.01562 0.00000 0.01562 1.87348

A7 1.93146 0.00299 0.01494 0.00000 0.01494 1.94640

A8 1.94134 0.00017 -0.00012 0.00000 -0.00012 1.94122

A9 1.84636 -0.00143 -0.01399 0.00000 -0.01399 1.83238

A10 1.88007 -0.00112 -0.00758 0.00000 -0.00758 1.87248

A11 1.91449 -0.00040 -0.00153 0.00000 -0.00153 1.91296

A12 1.93072 -0.00021 -0.00427 0.00000 -0.00427 1.92646

A13 1.94396 0.00105 0.00825 0.00000 0.00825 1.95222

A14 1.88518 0.00005 -0.00169 0.00000 -0.00169 1.88349

A15 1.88819 0.00012 0.00596 0.00000 0.00596 1.89416

A16 1.89983 -0.00064 -0.00688 0.00000 -0.00688 1.89295

A17 1.79441 0.00217 0.00431 0.00000 0.00431 1.79871

A18 1.97505 -0.00141 -0.00480 0.00000 -0.00480 1.97024

A19 2.14280 0.00133 0.00013 0.00000 0.00013 2.14293

A20 2.15306 0.00012 0.00202 0.00000 0.00202 2.15509

A21 1.80592 -0.00259 -0.01016 0.00000 -0.01016 1.79575

A22 1.93496 -0.00210 -0.00829 0.00000 -0.00829 1.92668

A23 1.88005 0.00078 -0.00090 0.00000 -0.00090 1.87915

A24 1.88273 0.00097 0.00919 0.00000 0.00919 1.89192

A25 1.93977 0.00016 -0.00048 0.00000 -0.00048 1.93929

A26 1.93727 0.00044 0.00084 0.00000 0.00084 1.93812

A27 1.88679 -0.00017 0.00002 0.00000 0.00002 1.88681

A28 1.95056 0.00047 0.00238 0.00000 0.00238 1.95294

A29 1.91744 -0.00024 -0.00136 0.00000 -0.00136 1.91607

A30 1.92357 -0.00057 -0.00636 0.00000 -0.00636 1.91721

A31 1.90498 0.00002 0.00194 0.00000 0.00194 1.90691

A32 1.90651 0.00015 0.00190 0.00000 0.00190 1.90841

A33 1.85840 0.00016 0.00153 0.00000 0.00153 1.85993

A34 1.96669 -0.00032 -0.00063 0.00000 -0.00063 1.96606

A35 1.90841 0.00001 -0.00223 0.00000 -0.00223 1.90618

A36 1.90493 0.00024 0.00288 0.00000 0.00288 1.90782

A37 1.91314 0.00014 -0.00032 0.00000 -0.00032 1.91282

A38 1.91231 0.00003 0.00051 0.00000 0.00051 1.91282

A39 1.85498 -0.00008 -0.00019 0.00000 -0.00019 1.85479

A40 1.94737 -0.00013 -0.00181 0.00000 -0.00181 1.94556

A41 1.93891 0.00041 0.00314 0.00000 0.00314 1.94205

A42 1.94256 -0.00022 0.00026 0.00000 0.00026 1.94283

A43 1.87920 -0.00020 -0.00222 0.00000 -0.00222 1.87697

A44 1.87790 0.00005 -0.00077 0.00000 -0.00077 1.87713

A45 1.87461 0.00008 0.00131 0.00000 0.00131 1.87591

D1 2.60785 -0.00020 0.10768 0.00000 0.10768 2.71552

D2 -1.52445 0.00128 0.11324 0.00000 0.11323 -1.41122

D3 0.43350 -0.00015 0.09737 0.00000 0.09737 0.53087

D4 -0.56500 -0.00031 0.10307 0.00000 0.10307 -0.46194

D5 1.58588 0.00117 0.10862 0.00000 0.10862 1.69450

D6 -2.73935 -0.00026 0.09276 0.00000 0.09276 -2.64659

D7 -3.09698 -0.00016 -0.00328 0.00000 -0.00328 -3.10026

D8 0.01435 -0.00030 -0.00779 0.00000 -0.00779 0.00657

D9 -3.14153 -0.00020 -0.00256 0.00000 -0.00256 3.13910

D10 -1.06367 -0.00052 -0.00821 0.00000 -0.00821 -1.07188

D11 1.05176 -0.00076 -0.01432 0.00000 -0.01432 1.03745

D12 1.03661 0.00062 0.00812 0.00000 0.00812 1.04472

D13 3.11446 0.00030 0.00246 0.00000 0.00246 3.11692

D14 -1.05329 0.00006 -0.00364 0.00000 -0.00364 -1.05693

D15 -1.01050 0.00041 0.01614 0.00000 0.01614 -0.99435

D16 1.06736 0.00009 0.01049 0.00000 0.01049 1.07785

D17 -3.10040 -0.00015 0.00439 0.00000 0.00439 -3.09601

D18 -3.08707 0.00090 -0.00052 0.00000 -0.00052 -3.08759

D19 -0.87454 -0.00080 -0.00542 0.00000 -0.00542 -0.87995

D20 1.23010 0.00018 -0.00592 0.00000 -0.00592 1.22418

D21 1.81449 0.00060 0.00805 0.00000 0.00805 1.82255

D22 -1.16439 0.00040 0.02444 0.00000 0.02444 -1.13995

D23 2.58367 -0.00018 0.00880 0.00000 0.00880 2.59247

D24 -0.72173 0.00015 -0.00793 0.00000 -0.00793 -0.72966

D25 -3.08912 0.00049 0.05729 0.00000 0.05729 -3.03183

D26 -0.96329 -0.00010 0.05111 0.00000 0.05111 -0.91218

D27 1.06958 0.00061 0.05544 0.00000 0.05544 1.12502

D28 -3.13744 -0.00012 0.01278 0.00000 0.01278 -3.12467

D29 -1.02018 0.00005 0.01587 0.00000 0.01587 -1.00431

D30 1.02229 -0.00023 0.01318 0.00000 0.01318 1.03547

D31 1.05527 0.00019 0.01966 0.00000 0.01966 1.07494

D32 -3.11065 0.00036 0.02276 0.00000 0.02276 -3.08789

D33 -1.06818 0.00007 0.02007 0.00000 0.02007 -1.04811

D34 -1.04524 0.00000 0.01940 0.00000 0.01940 -1.02585

D35 1.07202 0.00017 0.02249 0.00000 0.02249 1.09451

D36 3.11449 -0.00011 0.01980 0.00000 0.01980 3.13429

D37 3.13134 0.00017 0.01899 0.00000 0.01899 -3.13285

D38 -1.01969 0.00013 0.01657 0.00000 0.01657 -1.00312

D39 1.00272 0.00017 0.01671 0.00000 0.01671 1.01944

D40 1.00689 0.00015 0.01782 0.00000 0.01782 1.02470

D41 3.13904 0.00011 0.01540 0.00000 0.01540 -3.12875

D42 -1.12174 0.00015 0.01554 0.00000 0.01554 -1.10619

D43 -1.01858 -0.00013 0.01383 0.00000 0.01383 -1.00475

D44 1.11357 -0.00017 0.01141 0.00000 0.01141 1.12499

D45 3.13598 -0.00013 0.01156 0.00000 0.01156 -3.13565

D46 3.12025 -0.00004 0.01606 0.00000 0.01606 3.13631

D47 -1.06581 -0.00010 0.01415 0.00000 0.01415 -1.05166

D48 1.02228 0.00013 0.01809 0.00000 0.01809 1.04036

D49 0.99077 0.00007 0.01956 0.00000 0.01956 1.01033

D50 3.08789 0.00001 0.01765 0.00000 0.01765 3.10554

D51 -1.10721 0.00024 0.02159 0.00000 0.02159 -1.08562

D52 -1.03849 0.00007 0.01968 0.00000 0.01968 -1.01881

D53 1.05864 0.00001 0.01777 0.00000 0.01777 1.07641

D54 -3.13646 0.00024 0.02170 0.00000 0.02170 -3.11475

Item Value Threshold Converged?

Maximum Force 0.007455 0.000450 NO

RMS Force 0.001090 0.000300 NO

Maximum Displacement 0.360159 0.001800 NO

RMS Displacement 0.067931 0.001200 NO

Predicted change in Energy=-2.878188D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:56:00 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.095446 -0.405638 -0.205195

2 6 0 -2.845042 0.073908 0.472054

3 8 0 -4.889926 0.310840 -0.773389

4 8 0 -4.244329 -1.747856 -0.164396

5 6 0 -2.299268 -0.812928 1.574001

6 16 0 -1.578275 0.295729 -0.941279

7 6 0 -0.116545 0.765999 -0.093202

8 16 0 1.082639 -0.561926 0.018361

9 16 0 0.022190 2.246443 0.774984

10 6 0 2.687687 0.332381 -0.002827

11 6 0 3.846100 -0.656737 -0.070718

12 6 0 5.203545 0.052345 -0.066082

13 6 0 6.376558 -0.922522 -0.145959

14 1 0 -3.039399 1.081532 0.836793

15 1 0 -5.054335 -1.963696 -0.656515

16 1 0 -1.393926 -0.367066 1.987972

17 1 0 -3.029227 -0.906926 2.384330

18 1 0 -2.058045 -1.811480 1.209211

19 1 0 2.685837 0.996316 -0.870258

20 1 0 2.750521 0.947843 0.894749

21 1 0 3.795481 -1.346539 0.780186

22 1 0 3.759682 -1.269490 -0.975311

23 1 0 5.248353 0.751483 -0.909461

24 1 0 5.291877 0.660325 0.841964

25 1 0 7.335647 -0.395919 -0.146716

26 1 0 6.379056 -1.611597 0.705017

27 1 0 6.330751 -1.526460 -1.058092

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.500713 0.000000

3 O 1.211356 2.405996 0.000000

4 O 1.351066 2.383672 2.241852 0.000000

5 C 2.560797 1.516124 3.672139 2.771169 0.000000

6 S 2.714753 1.910868 3.315938 3.447844 2.841757

7 C 4.149329 2.871098 4.843035 4.833543 3.168099

8 S 5.185265 4.004598 6.087702 5.460441 3.730993

9 S 4.994919 3.610083 5.502082 5.919463 3.922671

10 C 6.826165 5.559084 7.616721 7.239222 5.354235

11 C 7.946652 6.752764 8.817488 8.164211 6.363571

12 C 9.311302 8.066587 10.121525 9.618353 7.728568

13 C 10.484920 9.295844 11.351145 10.652922 8.845350

14 H 2.100630 1.089089 2.571206 3.234141 2.163388

15 H 1.884331 3.210369 2.283463 0.972049 3.726911

16 H 3.479896 2.144342 4.506294 3.829368 1.090783

17 H 2.844952 2.157025 3.862169 2.946123 1.094673

18 H 2.850954 2.171970 4.056414 2.582766 1.090123

19 H 6.956550 5.765697 7.607328 7.487050 5.839437

20 H 7.064634 5.679152 7.846329 7.570766 5.390924

21 H 8.007684 6.797732 8.977571 8.105049 6.169347

22 H 7.939922 6.893618 8.795109 8.059194 6.589258

23 H 9.441478 8.238370 10.148762 9.844431 8.098243

24 H 9.505507 8.166406 10.315068 9.886927 7.767357

25 H 11.431247 10.210291 12.262008 11.658639 9.796241

26 H 10.582912 9.379722 11.526986 10.659772 8.758214

27 H 10.520896 9.439158 11.373667 10.615084 9.050650

6 7 8 9 10

6 S 0.000000

7 C 1.754151 0.000000

8 S 2.955832 1.792728 0.000000

9 S 3.051612 1.721833 3.095798 0.000000

10 C 4.368120 2.838998 1.837502 3.372461 0.000000

11 C 5.575743 4.210372 2.766521 4.875033 1.524757

12 C 6.842390 5.367811 4.167293 5.689279 2.532186

13 C 8.086782 6.709268 5.308729 7.160200 3.899107

14 H 2.431853 3.083428 4.512425 3.276304 5.836583

15 H 4.155608 5.670126 6.331103 6.748746 8.101740

16 H 3.008952 2.691992 3.170286 3.210475 4.594787

17 H 3.822475 4.173794 4.756498 4.673850 6.318030

18 H 3.048789 3.479813 3.583770 4.580685 5.346695

19 H 4.321865 2.917226 2.405827 3.371150 1.092359

20 H 4.747076 3.037957 2.414392 3.023986 1.090130

21 H 5.876882 4.530957 2.924980 5.210304 2.158492

22 H 5.562811 4.466148 2.941869 5.421639 2.158910

23 H 6.841899 5.426658 4.465319 5.690785 2.748571

24 H 7.107171 5.489694 4.459810 5.503622 2.757358

25 H 8.975952 7.542419 6.257389 7.830597 4.706873

26 H 8.346694 6.962970 5.442917 7.436337 4.231584

27 H 8.117063 6.910427 5.443506 7.575810 4.223836

11 12 13 14 15

11 C 0.000000

12 C 1.531495 0.000000

13 C 2.545490 1.527319 0.000000

14 H 7.159277 8.355869 9.676894 0.000000

15 H 9.014934 10.470776 11.489562 3.945041 0.000000

16 H 5.637374 6.922548 8.077290 2.476132 4.789690

17 H 7.304791 8.643104 9.740194 2.519711 3.803231

18 H 6.150656 7.604663 8.588903 3.077543 3.532967

19 H 2.172109 2.806535 4.222318 5.974915 8.289609

20 H 2.169584 2.782524 4.210639 5.791753 8.473444

21 H 1.096552 2.157705 2.774796 7.253573 8.986892

22 H 1.096003 2.158399 2.766993 7.418796 8.847060

23 H 2.157055 1.096399 2.158257 8.476153 10.657465

24 H 2.158220 1.096353 2.158223 8.341919 10.778452

25 H 3.500106 2.180206 1.094149 10.525765 12.499179

26 H 2.815917 2.178330 1.094984 9.796816 11.519556

27 H 2.811550 2.178830 1.094909 9.909183 11.400554

16 17 18 19 20

16 H 0.000000

17 H 1.767132 0.000000

18 H 1.770270 1.772658 0.000000

19 H 5.164567 6.846651 5.891716 0.000000

20 H 4.483365 6.250160 5.552932 1.766857 0.000000

21 H 5.417385 7.024469 5.887614 3.073148 2.523738

22 H 6.012911 7.583398 6.237936 2.509593 3.071172

23 H 7.332540 9.061882 8.027515 2.574484 3.087539

24 H 6.860673 8.606738 7.763121 3.136246 2.558114

25 H 8.986833 10.681663 9.596030 4.907399 4.890166

26 H 7.975844 9.582924 8.454516 4.787752 4.444434

27 H 8.384112 9.992160 8.694469 4.436787 4.770095

21 22 23 24 25

21 H 0.000000

22 H 1.757551 0.000000

23 H 3.060627 2.510938 0.000000

24 H 2.504101 3.061747 1.754335 0.000000

25 H 3.780952 3.773223 2.501021 2.504023 0.000000

26 H 2.598224 3.130759 3.077202 2.522368 1.765895

27 H 3.136754 2.585204 2.526400 3.077579 1.765940

26 27

26 H 0.000000

27 H 1.765824 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 9.06D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.104427 -0.463757 -0.129769

2 6 0 -2.848669 0.119150 0.449395

3 8 0 -4.903035 0.150197 -0.802576

4 8 0 -4.253434 -1.780520 0.133508

5 6 0 -2.294691 -0.574175 1.678640

6 16 0 -1.592785 0.102224 -0.990704

7 6 0 -0.124391 0.703887 -0.243133

8 16 0 1.075179 -0.589243 0.077371

9 16 0 0.021539 2.307268 0.367262

10 6 0 2.680312 0.286679 -0.103526

11 6 0 3.837837 -0.701909 -0.015709

12 6 0 5.195513 -0.003997 -0.138641

13 6 0 6.367551 -0.980536 -0.065111

14 1 0 -3.039868 1.173519 0.643979

15 1 0 -5.067291 -2.073449 -0.310011

16 1 0 -1.386030 -0.067461 2.006336

17 1 0 -3.018398 -0.531740 2.498857

18 1 0 -2.056625 -1.619682 1.482151

19 1 0 2.671980 0.798069 -1.068751

20 1 0 2.750283 1.041963 0.679439

21 1 0 3.793566 -1.241460 0.937890

22 1 0 3.744231 -1.455644 -0.805863

23 1 0 5.234036 0.546014 -1.086319

24 1 0 5.291060 0.745598 0.655693

25 1 0 7.326779 -0.462844 -0.160179

26 1 0 6.376395 -1.519442 0.888037

27 1 0 6.314498 -1.726888 -0.864467

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3049091 0.1933848 0.1808648

Leave Link 202 at Sat Aug 17 17:56:00 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.3074231527 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0549985629 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.2524245898 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2321

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.41D-09

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 97

GePol: Fraction of low-weight points (<1% of avg) = 4.18%

GePol: Cavity surface area = 309.217 Ang\*\*2

GePol: Cavity volume = 320.405 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057853288 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.2466392610 Hartrees.

Leave Link 301 at Sat Aug 17 17:56:00 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:56:00 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:56:00 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Lowest energy guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000118 -0.000021 -0.000015 Ang= -0.01 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999989 0.004587 0.000944 0.000675 Ang= 0.54 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 1.96D-02

Max alpha theta= 4.926 degrees.

Max beta theta= 5.019 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 17:56:01 2019, MaxMem= 1342177280 cpu: 4.3

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16161123.

Iteration 1 A\*A^-1 deviation from unit magnitude is 4.88D-15 for 2311.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.23D-15 for 2285 19.

Iteration 1 A^-1\*A deviation from unit magnitude is 4.88D-15 for 2311.

Iteration 1 A^-1\*A deviation from orthogonality is 1.31D-09 for 804 797.

Iteration 2 A\*A^-1 deviation from unit magnitude is 3.00D-15 for 338.

Iteration 2 A\*A^-1 deviation from orthogonality is 3.03D-15 for 1463 1123.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 1265.

Iteration 2 A^-1\*A deviation from orthogonality is 5.24D-16 for 2293 180.

E= -1658.67701775545

DIIS: error= 2.34D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67701775545 IErMin= 1 ErrMin= 2.34D-05

ErrMax= 2.34D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.31D-07 BMatP= 2.31D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 88.637 Goal= None Shift= 0.000

Gap= 88.629 Goal= None Shift= 0.000

RMSDP=9.70D-07 MaxDP=6.85D-05 OVMax= 9.66D-05

Cycle 2 Pass 1 IDiag 1:

RMSU= 9.68D-07 CP: 1.00D+00

E= -1658.67701773791 Delta-E= 0.000000017546 Rises=F Damp=F

DIIS: error= 2.24D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 1 EnMin= -1658.67701775545 IErMin= 2 ErrMin= 2.24D-05

ErrMax= 2.24D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.78D-07 BMatP= 2.31D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.569D+00 0.431D+00

Coeff: 0.569D+00 0.431D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=7.35D-07 MaxDP=5.27D-05 DE= 1.75D-08 OVMax= 6.53D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 4.35D-07 CP: 1.00D+00 3.91D-01

E= -1658.67701780175 Delta-E= -0.000000063840 Rises=F Damp=F

DIIS: error= 4.56D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67701780175 IErMin= 3 ErrMin= 4.56D-06

ErrMax= 4.56D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.07D-08 BMatP= 2.31D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.819D-01 0.197D+00 0.721D+00

Coeff: 0.819D-01 0.197D+00 0.721D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.36D-07 MaxDP=1.22D-05 DE=-6.38D-08 OVMax= 2.59D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.68D-07 CP: 1.00D+00 4.88D-01 6.87D-01

E= -1658.67701780374 Delta-E= -0.000000001997 Rises=F Damp=F

DIIS: error= 4.57D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67701780374 IErMin= 3 ErrMin= 4.56D-06

ErrMax= 4.57D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.22D-09 BMatP= 2.07D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.469D-02 0.888D-01 0.492D+00 0.424D+00

Coeff: -0.469D-02 0.888D-01 0.492D+00 0.424D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.09D-07 MaxDP=4.43D-06 DE=-2.00D-09 OVMax= 1.27D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.39D-08 CP: 1.00D+00 4.85D-01 8.07D-01 4.69D-01

E= -1658.67701780548 Delta-E= -0.000000001732 Rises=F Damp=F

DIIS: error= 5.34D-07 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67701780548 IErMin= 5 ErrMin= 5.34D-07

ErrMax= 5.34D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.33D-10 BMatP= 9.22D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.801D-02 0.341D-01 0.213D+00 0.218D+00 0.543D+00

Coeff: -0.801D-02 0.341D-01 0.213D+00 0.218D+00 0.543D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.98D-08 MaxDP=1.19D-06 DE=-1.73D-09 OVMax= 1.54D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.27D-08 CP: 1.00D+00 4.87D-01 8.13D-01 4.83D-01 5.64D-01

E= -1658.67701780546 Delta-E= 0.000000000015 Rises=F Damp=F

DIIS: error= 9.27D-08 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 5 EnMin= -1658.67701780548 IErMin= 6 ErrMin= 9.27D-08

ErrMax= 9.27D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.25D-11 BMatP= 2.33D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.256D-02 0.738D-02 0.511D-01 0.558D-01 0.241D+00 0.647D+00

Coeff: -0.256D-02 0.738D-02 0.511D-01 0.558D-01 0.241D+00 0.647D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.67D-09 MaxDP=3.37D-07 DE= 1.50D-11 OVMax= 5.36D-07

Error on total polarization charges = 0.04162

SCF Done: E(UB3LYP) = -1658.67701781 A.U. after 6 cycles

NFock= 6 Conv=0.57D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655236256609D+03 PE=-6.147259125555D+03 EE= 1.731099211880D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.63

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:56:16 2019, MaxMem= 1342177280 cpu: 174.5

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 335

Leave Link 701 at Sat Aug 17 17:56:17 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:56:17 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:56:21 2019, MaxMem= 1342177280 cpu: 38.5

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.40829093D+00-2.94672373D+00 6.34315209D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000102475 -0.000079532 0.000101829

2 6 -0.000043025 -0.000078973 -0.000025162

3 8 -0.000118120 0.000210080 -0.000044020

4 8 0.000109393 -0.000058425 0.000019358

5 6 -0.000034906 -0.000047576 0.000018918

6 16 -0.000026637 0.000053446 0.000006332

7 6 0.000029455 0.000038623 0.000027537

8 16 0.000014771 -0.000008001 0.000001145

9 16 -0.000018956 -0.000031614 0.000074120

10 6 0.000003267 0.000001032 0.000022676

11 6 -0.000017780 -0.000005600 -0.000018286

12 6 0.000003424 0.000021047 -0.000010861

13 6 -0.000001230 -0.000012293 -0.000012316

14 1 0.000015195 0.000019337 0.000004873

15 1 -0.000016791 0.000051783 -0.000046189

16 1 -0.000000009 -0.000034274 0.000001877

17 1 0.000008942 -0.000055646 -0.000012486

18 1 0.000001341 -0.000043695 -0.000036600

19 1 0.000027716 0.000032659 0.000019719

20 1 -0.000029682 -0.000020376 0.000042269

21 1 -0.000006578 -0.000014169 -0.000029220

22 1 -0.000008025 0.000014114 -0.000036280

23 1 0.000002474 0.000039567 0.000010229

24 1 0.000005532 -0.000018884 0.000017696

25 1 0.000000329 0.000010682 -0.000008567

26 1 0.000001445 -0.000028601 -0.000043175

27 1 -0.000004021 0.000045288 -0.000045415

-------------------------------------------------------------------

Cartesian Forces: Max 0.000210080 RMS 0.000044767

Leave Link 716 at Sat Aug 17 17:56:21 2019, MaxMem= 1342177280 cpu: 0.3

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000216009 RMS 0.000031280

Search for a local minimum.

Step number 57 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .31280D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43 45 44 47 46

49 48 51 50 53

54 55 56 52 57

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 1 1 1 -1 -1

ITU= 0 -1 -1 -1 0 -1 0 0 -1 -1 0 0 -1 0 0 -1 1 -1 1 -1

ITU= 1 1 -1 1 -1 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Use linear search instead of GDIIS.

Eigenvalues --- 0.00000 0.00009 0.00050 0.00120 0.00307

Eigenvalues --- 0.00327 0.00455 0.00529 0.01210 0.01842

Eigenvalues --- 0.02499 0.03305 0.03517 0.03688 0.04008

Eigenvalues --- 0.04497 0.04689 0.04785 0.04968 0.05233

Eigenvalues --- 0.05431 0.05437 0.05666 0.06030 0.06298

Eigenvalues --- 0.08237 0.08304 0.10587 0.10854 0.11257

Eigenvalues --- 0.11905 0.13666 0.14285 0.15361 0.15679

Eigenvalues --- 0.15941 0.16113 0.16314 0.16535 0.17477

Eigenvalues --- 0.18183 0.19325 0.20103 0.21817 0.21985

Eigenvalues --- 0.22503 0.23420 0.24850 0.25541 0.25881

Eigenvalues --- 0.26672 0.28543 0.29041 0.29375 0.29455

Eigenvalues --- 0.30099 0.31782 0.33004 0.33780 0.33852

Eigenvalues --- 0.33913 0.33951 0.34010 0.34036 0.34072

Eigenvalues --- 0.34128 0.34148 0.34220 0.34670 0.35040

Eigenvalues --- 0.35879 0.40101 0.47507 0.53030 0.90953

RFO step: Lambda=-7.65078224D-06 EMin= 2.70524123D-06

Quartic linear search produced a step of -0.65755.

Iteration 1 RMS(Cart)= 0.10353337 RMS(Int)= 0.00466872

Iteration 2 RMS(Cart)= 0.00929743 RMS(Int)= 0.00007176

Iteration 3 RMS(Cart)= 0.00005116 RMS(Int)= 0.00006536

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00006536

ITry= 1 IFail=0 DXMaxC= 4.31D-01 DCOld= 1.00D+10 DXMaxT= 1.20D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83594 -0.00011 -0.00015 -0.02389 -0.02404 2.81190

R2 2.28913 0.00022 0.00012 0.00448 0.00459 2.29373

R3 2.55315 0.00004 0.00001 -0.01658 -0.01657 2.53658

R4 2.86506 0.00002 0.00001 0.01332 0.01333 2.87839

R5 3.61102 0.00000 -0.00023 0.02815 0.02792 3.63893

R6 2.05808 0.00002 -0.00001 0.00958 0.00957 2.06765

R7 1.83691 0.00001 0.00002 0.00222 0.00223 1.83914

R8 2.06128 0.00000 -0.00003 0.00968 0.00965 2.07094

R9 2.06863 -0.00001 -0.00001 0.00687 0.00686 2.07550

R10 2.06003 0.00002 0.00001 0.00051 0.00052 2.06056

R11 3.31486 0.00000 0.00019 0.00041 0.00060 3.31546

R12 3.38777 0.00001 -0.00007 0.02514 0.02506 3.41283

R13 3.25379 -0.00001 0.00004 0.01538 0.01543 3.26922

R14 3.47238 -0.00002 -0.00006 -0.01310 -0.01316 3.45922

R15 2.88137 -0.00001 0.00000 0.00751 0.00751 2.88888

R16 2.06426 0.00001 0.00000 0.00312 0.00312 2.06738

R17 2.06005 0.00001 0.00002 0.00022 0.00024 2.06029

R18 2.89411 0.00002 0.00001 0.00646 0.00648 2.90058

R19 2.07218 0.00000 0.00001 0.00299 0.00300 2.07518

R20 2.07115 0.00001 -0.00001 0.00552 0.00551 2.07666

R21 2.88622 0.00001 0.00001 -0.00370 -0.00369 2.88252

R22 2.07189 0.00002 0.00001 0.00578 0.00579 2.07768

R23 2.07181 0.00000 -0.00001 0.00329 0.00328 2.07509

R24 2.06764 0.00000 0.00000 0.00386 0.00386 2.07150

R25 2.06922 0.00001 0.00001 0.00530 0.00531 2.07453

R26 2.06908 0.00000 -0.00001 0.00269 0.00268 2.07176

A1 2.17626 -0.00002 0.00001 -0.00251 -0.00251 2.17375

A2 1.97756 -0.00010 -0.00004 0.00153 0.00148 1.97905

A3 2.12879 0.00012 0.00003 0.00073 0.00075 2.12954

A4 2.02754 -0.00005 -0.00004 -0.00930 -0.00940 2.01814

A5 1.82933 0.00002 -0.00020 0.01406 0.01388 1.84321

A6 1.87348 0.00001 0.00020 -0.03071 -0.03039 1.84310

A7 1.94640 0.00004 0.00020 0.01408 0.01419 1.96059

A8 1.94122 0.00002 0.00000 0.02589 0.02576 1.96698

A9 1.83238 -0.00004 -0.00018 -0.01697 -0.01729 1.81508

A10 1.87248 -0.00005 -0.00010 -0.00696 -0.00706 1.86542

A11 1.91296 -0.00002 -0.00002 -0.01478 -0.01482 1.89814

A12 1.92646 0.00000 -0.00006 0.00106 0.00096 1.92742

A13 1.95222 0.00001 0.00011 0.00600 0.00608 1.95830

A14 1.88349 0.00000 -0.00002 0.00183 0.00178 1.88527

A15 1.89416 0.00001 0.00008 -0.00403 -0.00396 1.89020

A16 1.89295 0.00000 -0.00009 0.00994 0.00980 1.90275

A17 1.79871 -0.00008 0.00006 -0.00089 -0.00084 1.79788

A18 1.97024 -0.00002 -0.00006 -0.00749 -0.00757 1.96267

A19 2.14293 -0.00002 0.00000 0.00080 0.00078 2.14371

A20 2.15509 0.00003 0.00003 0.00485 0.00485 2.15994

A21 1.79575 0.00003 -0.00013 0.01184 0.01170 1.80746

A22 1.92668 -0.00003 -0.00011 0.01582 0.01567 1.94235

A23 1.87915 0.00004 -0.00001 -0.01150 -0.01160 1.86755

A24 1.89192 -0.00002 0.00012 -0.01063 -0.01060 1.88132

A25 1.93929 -0.00002 -0.00001 0.00651 0.00652 1.94581

A26 1.93812 0.00003 0.00001 0.00633 0.00635 1.94447

A27 1.88681 0.00000 0.00000 -0.00793 -0.00802 1.87879

A28 1.95294 0.00000 0.00003 -0.01710 -0.01717 1.93577

A29 1.91607 -0.00001 -0.00002 -0.00645 -0.00671 1.90936

A30 1.91721 0.00000 -0.00008 0.01833 0.01828 1.93549

A31 1.90691 0.00000 0.00003 -0.00718 -0.00737 1.89955

A32 1.90841 0.00000 0.00003 0.00245 0.00259 1.91100

A33 1.85993 0.00000 0.00002 0.01126 0.01129 1.87122

A34 1.96606 -0.00001 -0.00001 0.00494 0.00491 1.97097

A35 1.90618 0.00001 -0.00003 -0.00027 -0.00033 1.90585

A36 1.90782 0.00000 0.00004 -0.00430 -0.00428 1.90354

A37 1.91282 0.00000 0.00000 0.00605 0.00604 1.91887

A38 1.91282 0.00000 0.00001 -0.01168 -0.01166 1.90116

A39 1.85479 0.00000 0.00000 0.00529 0.00531 1.86011

A40 1.94556 -0.00001 -0.00002 -0.01352 -0.01357 1.93199

A41 1.94205 0.00001 0.00004 -0.00657 -0.00657 1.93548

A42 1.94283 -0.00001 0.00000 0.00553 0.00556 1.94838

A43 1.87697 0.00000 -0.00003 0.00585 0.00574 1.88271

A44 1.87713 0.00001 -0.00001 0.01557 0.01559 1.89273

A45 1.87591 0.00000 0.00002 -0.00591 -0.00589 1.87003

D1 2.71552 -0.00002 0.00142 -0.13647 -0.13493 2.58059

D2 -1.41122 0.00001 0.00149 -0.11358 -0.11208 -1.52330

D3 0.53087 -0.00002 0.00128 -0.13893 -0.13780 0.39307

D4 -0.46194 -0.00003 0.00136 -0.14421 -0.14273 -0.60466

D5 1.69450 0.00000 0.00143 -0.12132 -0.11987 1.57464

D6 -2.64659 -0.00002 0.00122 -0.14667 -0.14559 -2.79218

D7 -3.10026 0.00000 -0.00004 0.09535 0.09531 -3.00495

D8 0.00657 0.00000 -0.00010 0.08777 0.08766 0.09423

D9 3.13910 0.00001 -0.00003 0.04368 0.04370 -3.10039

D10 -1.07188 0.00000 -0.00011 0.03743 0.03737 -1.03451

D11 1.03745 0.00001 -0.00019 0.05482 0.05470 1.09215

D12 1.04472 0.00000 0.00011 0.02056 0.02075 1.06547

D13 3.11692 -0.00001 0.00003 0.01431 0.01443 3.13135

D14 -1.05693 -0.00001 -0.00005 0.03170 0.03175 -1.02518

D15 -0.99435 0.00000 0.00021 0.01629 0.01635 -0.97800

D16 1.07785 0.00000 0.00014 0.01004 0.01003 1.08787

D17 -3.09601 0.00000 0.00006 0.02743 0.02735 -3.06865

D18 -3.08759 0.00003 -0.00001 -0.03017 -0.03026 -3.11785

D19 -0.87995 0.00000 -0.00007 -0.02333 -0.02319 -0.90315

D20 1.22418 0.00002 -0.00008 0.00505 0.00485 1.22903

D21 1.82255 -0.00003 0.00011 -0.01323 -0.01311 1.80943

D22 -1.13995 0.00004 0.00032 -0.00273 -0.00242 -1.14237

D23 2.59247 0.00005 0.00012 0.03438 0.03451 2.62698

D24 -0.72966 -0.00002 -0.00010 0.02331 0.02319 -0.70646

D25 -3.03183 0.00000 0.00075 -0.02633 -0.02557 -3.05740

D26 -0.91218 -0.00002 0.00067 -0.01610 -0.01555 -0.92773

D27 1.12502 -0.00001 0.00073 -0.03714 -0.03629 1.08873

D28 -3.12467 0.00001 0.00017 0.12379 0.12389 -3.00078

D29 -1.00431 0.00001 0.00021 0.09880 0.09904 -0.90526

D30 1.03547 0.00001 0.00017 0.11943 0.11963 1.15510

D31 1.07494 0.00000 0.00026 0.12366 0.12383 1.19877

D32 -3.08789 0.00000 0.00030 0.09867 0.09898 -2.98891

D33 -1.04811 -0.00001 0.00026 0.11930 0.11957 -0.92854

D34 -1.02585 -0.00001 0.00026 0.12506 0.12527 -0.90058

D35 1.09451 -0.00001 0.00030 0.10007 0.10042 1.19493

D36 3.13429 -0.00001 0.00026 0.12070 0.12101 -3.02789

D37 -3.13285 0.00000 0.00025 0.10275 0.10304 -3.02982

D38 -1.00312 0.00000 0.00022 0.11360 0.11385 -0.88926

D39 1.01944 0.00000 0.00022 0.11738 0.11764 1.13708

D40 1.02470 0.00000 0.00023 0.12713 0.12731 1.15202

D41 -3.12875 0.00000 0.00020 0.13798 0.13813 -2.99061

D42 -1.10619 0.00001 0.00020 0.14177 0.14192 -0.96427

D43 -1.00475 0.00000 0.00018 0.11629 0.11649 -0.88826

D44 1.12499 0.00000 0.00015 0.12714 0.12731 1.25229

D45 -3.13565 0.00000 0.00015 0.13093 0.13109 -3.00455

D46 3.13631 0.00001 0.00021 -0.08324 -0.08305 3.05326

D47 -1.05166 0.00001 0.00019 -0.08943 -0.08922 -1.14088

D48 1.04036 0.00001 0.00024 -0.09762 -0.09737 0.94300

D49 1.01033 0.00000 0.00026 -0.09055 -0.09034 0.91999

D50 3.10554 0.00000 0.00023 -0.09675 -0.09651 3.00903

D51 -1.08562 0.00000 0.00028 -0.10494 -0.10466 -1.19028

D52 -1.01881 0.00000 0.00026 -0.09371 -0.09347 -1.11228

D53 1.07641 0.00000 0.00023 -0.09991 -0.09964 0.97676

D54 -3.11475 0.00001 0.00029 -0.10810 -0.10780 3.06063

Item Value Threshold Converged?

Maximum Force 0.000216 0.000450 YES

RMS Force 0.000031 0.000300 YES

Maximum Displacement 0.431275 0.001800 NO

RMS Displacement 0.104717 0.001200 NO

Predicted change in Energy=-1.388255D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:56:21 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.121105 -0.399363 -0.116014

2 6 0 -2.843416 0.067813 0.486795

3 8 0 -4.981047 0.333162 -0.560070

4 8 0 -4.224165 -1.736315 -0.176858

5 6 0 -2.283657 -0.804604 1.602873

6 16 0 -1.613985 0.253038 -0.983674

7 6 0 -0.131265 0.763669 -0.196937

8 16 0 1.074872 -0.573902 -0.063743

9 16 0 0.023278 2.282045 0.617639

10 6 0 2.685563 0.294912 -0.105114

11 6 0 3.850081 -0.695360 -0.121597

12 6 0 5.190912 0.032881 0.045211

13 6 0 6.393453 -0.890910 -0.119844

14 1 0 -3.028684 1.097184 0.808111

15 1 0 -5.024573 -1.934835 -0.693688

16 1 0 -1.371437 -0.337684 1.991231

17 1 0 -3.004286 -0.880552 2.428221

18 1 0 -2.033825 -1.807659 1.255833

19 1 0 2.684922 0.927632 -0.997597

20 1 0 2.732894 0.950475 0.764748

21 1 0 3.731048 -1.412090 0.701835

22 1 0 3.860280 -1.272867 -1.056482

23 1 0 5.247986 0.856186 -0.681240

24 1 0 5.228325 0.491622 1.042187

25 1 0 7.328486 -0.319942 -0.083177

26 1 0 6.424571 -1.640151 0.681916

27 1 0 6.356933 -1.436026 -1.070345

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.487992 0.000000

3 O 1.213787 2.394954 0.000000

4 O 1.342298 2.366808 2.236617 0.000000

5 C 2.548531 1.523178 3.639883 2.793045 0.000000

6 S 2.732052 1.925640 3.394550 3.379574 2.873551

7 C 4.156683 2.882268 4.882375 4.796056 3.214278

8 S 5.199170 4.008475 6.143555 5.426214 3.756401

9 S 4.990401 3.624621 5.498037 5.900781 3.977441

10 C 6.841992 5.565208 7.680192 7.202456 5.368361

11 C 7.976682 6.764280 8.901626 8.141259 6.372478

12 C 9.323438 8.046530 10.194376 9.582435 7.680942

13 C 10.526042 9.306283 11.448642 10.651374 8.846888

14 H 2.070518 1.094154 2.503472 3.229250 2.191691

15 H 1.872868 3.187724 2.272346 0.973230 3.750232

16 H 3.464817 2.143473 4.470845 3.846406 1.095892

17 H 2.819922 2.166659 3.782932 3.001145 1.098305

18 H 2.867403 2.182717 4.070226 2.618260 1.090400

19 H 6.990000 5.788370 7.701422 7.450216 5.869400

20 H 7.040959 5.652574 7.851185 7.517057 5.380385

21 H 7.959322 6.742398 8.974348 8.010159 6.112085

22 H 8.083934 7.008471 8.999712 8.145353 6.711140

23 H 9.469728 8.213198 10.243112 9.833469 8.043695

24 H 9.462934 8.101919 10.335551 9.787714 7.643588

25 H 11.449913 10.195235 12.336068 11.639529 9.770924

26 H 10.648357 9.426070 11.641504 10.683740 8.796563

27 H 10.572355 9.451595 11.486523 10.623000 9.066674

6 7 8 9 10

6 S 0.000000

7 C 1.754468 0.000000

8 S 2.959739 1.805991 0.000000

9 S 3.059690 1.729995 3.118744 0.000000

10 C 4.388591 2.857041 1.830539 3.399828 0.000000

11 C 5.612366 4.240939 2.778468 4.904675 1.528730

12 C 6.885761 5.377570 4.161952 5.664880 2.523496

13 C 8.134733 6.731680 5.328315 7.154765 3.892922

14 H 2.434019 3.084865 4.515731 3.279428 5.842109

15 H 4.062387 5.610093 6.281099 6.706896 8.047632

16 H 3.042670 2.745739 3.203615 3.270316 4.610216

17 H 3.854736 4.224828 4.789932 4.737760 6.338287

18 H 3.072154 3.513119 3.595474 4.622190 5.342809

19 H 4.351537 2.932379 2.391432 3.395257 1.094011

20 H 4.736956 3.027068 2.399825 3.022704 1.090258

21 H 5.846621 4.523183 2.888588 5.234624 2.158255

22 H 5.683420 4.562754 3.038516 5.492055 2.177841

23 H 6.895063 5.401800 4.454361 5.569357 2.685696

24 H 7.139905 5.507690 4.428272 5.520723 2.796540

25 H 9.005942 7.538902 6.258799 7.786369 4.683510

26 H 8.424769 7.037735 5.505649 7.507616 4.282997

27 H 8.148373 6.906390 5.445794 7.535817 4.172143

11 12 13 14 15

11 C 0.000000

12 C 1.534923 0.000000

13 C 2.550879 1.525365 0.000000

14 H 7.169030 8.323252 9.674207 0.000000

15 H 8.979035 10.429478 11.480000 3.928373 0.000000

16 H 5.644133 6.854834 8.065744 2.491001 4.806775

17 H 7.315615 8.583378 9.737055 2.556716 3.865151

18 H 6.144500 7.553147 8.587894 3.102952 3.572308

19 H 2.181531 2.857974 4.222647 5.994549 8.229362

20 H 2.177726 2.720582 4.192003 5.763609 8.404186

21 H 1.098140 2.156456 2.834640 7.211223 8.881534

22 H 1.098921 2.165476 2.727664 7.520084 8.916862

23 H 2.162090 1.099463 2.163240 8.413056 10.644972

24 H 2.159369 1.098090 2.149240 8.282494 10.678150

25 H 3.498816 2.170297 1.096191 10.491597 12.473118

26 H 2.857667 2.174015 1.097793 9.842406 11.535251

27 H 2.780830 2.182145 1.096329 9.901291 11.398656

16 17 18 19 20

16 H 0.000000

17 H 1.775348 0.000000

18 H 1.772116 1.782081 0.000000

19 H 5.195014 6.882794 5.901385 0.000000

20 H 4.473159 6.247803 5.529022 1.763146 0.000000

21 H 5.371429 6.973354 5.804925 3.075183 2.565538

22 H 6.126499 7.708393 6.353997 2.495422 3.087252

23 H 7.237692 8.988047 7.992064 2.583502 2.902664

24 H 6.719025 8.460487 7.620444 3.289335 2.552390

25 H 8.943833 10.648360 9.573877 4.894415 4.842768

26 H 8.011770 9.619247 8.479498 4.837277 4.510729

27 H 8.384946 10.009043 8.715162 4.367590 4.711328

21 22 23 24 25

21 H 0.000000

22 H 1.768549 0.000000

23 H 3.059260 2.568930 0.000000

24 H 2.445771 3.064209 1.761673 0.000000

25 H 3.840650 3.726103 2.463623 2.517092 0.000000

26 H 2.703233 3.119698 3.078026 2.470881 1.773523

27 H 3.168039 2.502018 2.575928 3.074471 1.778780

26 27

26 H 0.000000

27 H 1.765407 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 7.33D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.118061 -0.446251 -0.065138

2 6 0 -2.839832 0.088771 0.477082

3 8 0 -4.980376 0.229360 -0.587863

4 8 0 -4.218811 -1.781551 0.027533

5 6 0 -2.275878 -0.649444 1.684172

6 16 0 -1.614167 0.106567 -1.008017

7 6 0 -0.130560 0.706107 -0.288561

8 16 0 1.078335 -0.605585 -0.006355

9 16 0 0.023093 2.307900 0.346683

10 6 0 2.687329 0.255306 -0.150848

11 6 0 3.853620 -0.728544 -0.056940

12 6 0 5.193498 0.016079 0.022133

13 6 0 6.397343 -0.918654 -0.039252

14 1 0 -3.026239 1.147841 0.679067

15 1 0 -5.020054 -2.039105 -0.461191

16 1 0 -1.363616 -0.139764 2.014298

17 1 0 -2.994445 -0.631649 2.514605

18 1 0 -2.025016 -1.685211 1.453460

19 1 0 2.683451 0.781832 -1.109814

20 1 0 2.735482 1.006099 0.638236

21 1 0 3.737818 -1.346610 0.843336

22 1 0 3.862702 -1.409138 -0.919689

23 1 0 5.247371 0.751013 -0.793826

24 1 0 5.232389 0.585859 0.960024

25 1 0 7.331410 -0.345784 -0.070463

26 1 0 6.431700 -1.571262 0.842831

27 1 0 6.359612 -1.568928 -0.921101

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3150392 0.1924683 0.1797691

Leave Link 202 at Sat Aug 17 17:56:21 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1099.8022787072 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0547320562 Hartrees.

Nuclear repulsion after empirical dispersion term = 1099.7475466510 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

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Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2330

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.12D-07

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 91

GePol: Fraction of low-weight points (<1% of avg) = 3.91%

GePol: Cavity surface area = 310.129 Ang\*\*2

GePol: Cavity volume = 321.334 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057764725 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1099.7417701785 Hartrees.

Leave Link 301 at Sat Aug 17 17:56:21 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.86D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:56:21 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:56:21 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999927 -0.012030 -0.000640 -0.000865 Ang= -1.38 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.62521892481

Leave Link 401 at Sat Aug 17 17:56:22 2019, MaxMem= 1342177280 cpu: 7.7

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16286700.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.77D-15 for 2309.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.39D-15 for 910 855.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.77D-15 for 2303.

Iteration 1 A^-1\*A deviation from orthogonality is 1.45D-10 for 2032 954.

Iteration 2 A\*A^-1 deviation from unit magnitude is 6.66D-15 for 385.

Iteration 2 A\*A^-1 deviation from orthogonality is 3.60D-15 for 961 22.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.44D-15 for 184.

Iteration 2 A^-1\*A deviation from orthogonality is 4.08D-16 for 2108 126.

E= -1658.64089178230

DIIS: error= 7.64D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.64089178230 IErMin= 1 ErrMin= 7.64D-03

ErrMax= 7.64D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.80D-02 BMatP= 7.80D-02

IDIUse=3 WtCom= 9.24D-01 WtEn= 7.64D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.430 Goal= None Shift= 0.000

Gap= 0.486 Goal= None Shift= 0.000

GapD= 0.430 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=5.60D-04 MaxDP=1.49D-02 OVMax= 3.69D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 5.60D-04 CP: 9.99D-01

E= -1658.67485095891 Delta-E= -0.033959176609 Rises=F Damp=F

DIIS: error= 1.06D-03 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67485095891 IErMin= 2 ErrMin= 1.06D-03

ErrMax= 1.06D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.04D-03 BMatP= 7.80D-02

IDIUse=3 WtCom= 9.89D-01 WtEn= 1.06D-02

Coeff-Com: -0.446D-01 0.104D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.441D-01 0.104D+01

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.132 Goal= None Shift= 0.000

RMSDP=1.28D-04 MaxDP=6.13D-03 DE=-3.40D-02 OVMax= 8.40D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.24D-04 CP: 9.99D-01 1.05D+00

E= -1658.67465210009 Delta-E= 0.000198858819 Rises=F Damp=F

DIIS: error= 1.91D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1658.67485095891 IErMin= 2 ErrMin= 1.06D-03

ErrMax= 1.91D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.03D-03 BMatP= 2.04D-03

IDIUse=3 WtCom= 1.86D-01 WtEn= 8.14D-01

Coeff-Com: -0.465D-01 0.643D+00 0.403D+00

Coeff-En: 0.000D+00 0.590D+00 0.410D+00

Coeff: -0.866D-02 0.600D+00 0.409D+00

Gap= 0.120 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=9.85D-05 MaxDP=5.89D-03 DE= 1.99D-04 OVMax= 8.68D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 4.66D-05 CP: 9.99D-01 1.08D+00 3.12D-01

E= -1658.67536914952 Delta-E= -0.000717049432 Rises=F Damp=F

DIIS: error= 6.81D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67536914952 IErMin= 4 ErrMin= 6.81D-04

ErrMax= 6.81D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.69D-04 BMatP= 2.04D-03

IDIUse=3 WtCom= 9.93D-01 WtEn= 6.81D-03

Coeff-Com: -0.151D-01 0.164D+00 0.254D+00 0.598D+00

Coeff-En: 0.000D+00 0.000D+00 0.893D-01 0.911D+00

Coeff: -0.150D-01 0.163D+00 0.252D+00 0.600D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.79D-05 MaxDP=1.29D-03 DE=-7.17D-04 OVMax= 2.37D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.38D-05 CP: 9.99D-01 1.08D+00 4.77D-01 7.28D-01

E= -1658.67543946210 Delta-E= -0.000070312575 Rises=F Damp=F

DIIS: error= 1.40D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67543946210 IErMin= 5 ErrMin= 1.40D-04

ErrMax= 1.40D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.56D-05 BMatP= 3.69D-04

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.40D-03

Coeff-Com: -0.504D-02 0.449D-01 0.115D+00 0.345D+00 0.500D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.503D-02 0.448D-01 0.115D+00 0.345D+00 0.500D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.64D-06 MaxDP=2.84D-04 DE=-7.03D-05 OVMax= 4.45D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.85D-06 CP: 9.99D-01 1.08D+00 4.76D-01 8.00D-01 6.94D-01

E= -1658.67544473868 Delta-E= -0.000005276582 Rises=F Damp=F

DIIS: error= 2.89D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67544473868 IErMin= 6 ErrMin= 2.89D-05

ErrMax= 2.89D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.90D-07 BMatP= 2.56D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.158D-03-0.805D-02 0.780D-02 0.461D-01 0.176D+00 0.778D+00

Coeff: 0.158D-03-0.805D-02 0.780D-02 0.461D-01 0.176D+00 0.778D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.09D-06 MaxDP=8.58D-05 DE=-5.28D-06 OVMax= 2.02D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.57D-06 CP: 9.99D-01 1.08D+00 4.78D-01 8.23D-01 7.50D-01

CP: 1.02D+00

E= -1658.67544488645 Delta-E= -0.000000147775 Rises=F Damp=F

DIIS: error= 1.52D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67544488645 IErMin= 7 ErrMin= 1.52D-05

ErrMax= 1.52D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.79D-07 BMatP= 8.90D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.508D-03-0.863D-02-0.497D-02-0.108D-02 0.629D-01 0.458D+00

Coeff-Com: 0.493D+00

Coeff: 0.508D-03-0.863D-02-0.497D-02-0.108D-02 0.629D-01 0.458D+00

Coeff: 0.493D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=9.08D-07 MaxDP=3.27D-05 DE=-1.48D-07 OVMax= 7.01D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 6.67D-07 CP: 9.99D-01 1.08D+00 4.79D-01 8.23D-01 7.76D-01

CP: 1.09D+00 7.70D-01

E= -1658.67544494896 Delta-E= -0.000000062510 Rises=F Damp=F

DIIS: error= 4.92D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67544494896 IErMin= 8 ErrMin= 4.92D-06

ErrMax= 4.92D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.22D-08 BMatP= 2.79D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.211D-03-0.289D-02-0.304D-02-0.545D-02 0.854D-02 0.114D+00

Coeff-Com: 0.232D+00 0.656D+00

Coeff: 0.211D-03-0.289D-02-0.304D-02-0.545D-02 0.854D-02 0.114D+00

Coeff: 0.232D+00 0.656D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.43D-07 MaxDP=2.32D-05 DE=-6.25D-08 OVMax= 8.20D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 3.23D-07 CP: 9.99D-01 1.08D+00 4.78D-01 8.27D-01 7.83D-01

CP: 1.14D+00 9.42D-01 9.36D-01

E= -1658.67544495518 Delta-E= -0.000000006219 Rises=F Damp=F

DIIS: error= 2.40D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67544495518 IErMin= 9 ErrMin= 2.40D-06

ErrMax= 2.40D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.04D-08 BMatP= 2.22D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.265D-04 0.923D-03-0.348D-03-0.330D-02-0.146D-01-0.715D-01

Coeff-Com: -0.169D-02 0.453D+00 0.638D+00

Coeff: -0.265D-04 0.923D-03-0.348D-03-0.330D-02-0.146D-01-0.715D-01

Coeff: -0.169D-02 0.453D+00 0.638D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.77D-07 MaxDP=1.32D-05 DE=-6.22D-09 OVMax= 3.53D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.05D-07 CP: 9.99D-01 1.08D+00 4.79D-01 8.28D-01 7.88D-01

CP: 1.17D+00 1.00D+00 1.20D+00 8.61D-01

E= -1658.67544495855 Delta-E= -0.000000003364 Rises=F Damp=F

DIIS: error= 6.90D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67544495855 IErMin=10 ErrMin= 6.90D-07

ErrMax= 6.90D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.34D-10 BMatP= 1.04D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.382D-04 0.768D-03 0.277D-03-0.771D-03-0.731D-02-0.453D-01

Coeff-Com: -0.358D-01 0.811D-01 0.251D+00 0.756D+00

Coeff: -0.382D-04 0.768D-03 0.277D-03-0.771D-03-0.731D-02-0.453D-01

Coeff: -0.358D-01 0.811D-01 0.251D+00 0.756D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.16D-07 MaxDP=4.42D-06 DE=-3.36D-09 OVMax= 1.32D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 5.74D-08 CP: 9.99D-01 1.08D+00 4.79D-01 8.29D-01 7.90D-01

CP: 1.18D+00 1.04D+00 1.26D+00 9.72D-01 8.78D-01

E= -1658.67544495889 Delta-E= -0.000000000340 Rises=F Damp=F

DIIS: error= 4.59D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67544495889 IErMin=11 ErrMin= 4.59D-07

ErrMax= 4.59D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.37D-10 BMatP= 7.34D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.148D-04 0.201D-03 0.222D-03 0.289D-03-0.653D-03-0.801D-02

Coeff-Com: -0.182D-01-0.561D-01-0.127D-01 0.413D+00 0.682D+00

Coeff: -0.148D-04 0.201D-03 0.222D-03 0.289D-03-0.653D-03-0.801D-02

Coeff: -0.182D-01-0.561D-01-0.127D-01 0.413D+00 0.682D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.23D-08 MaxDP=2.55D-06 DE=-3.40D-10 OVMax= 7.00D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 2.29D-08 CP: 9.99D-01 1.08D+00 4.79D-01 8.29D-01 7.90D-01

CP: 1.19D+00 1.06D+00 1.29D+00 1.03D+00 1.09D+00

CP: 8.54D-01

E= -1658.67544495898 Delta-E= -0.000000000096 Rises=F Damp=F

DIIS: error= 1.74D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1658.67544495898 IErMin=12 ErrMin= 1.74D-07

ErrMax= 1.74D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.51D-11 BMatP= 2.37D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.916D-06-0.572D-04 0.378D-04 0.247D-03 0.103D-02 0.503D-02

Coeff-Com: -0.925D-03-0.363D-01-0.494D-01 0.308D-01 0.270D+00 0.779D+00

Coeff: 0.916D-06-0.572D-04 0.378D-04 0.247D-03 0.103D-02 0.503D-02

Coeff: -0.925D-03-0.363D-01-0.494D-01 0.308D-01 0.270D+00 0.779D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.61D-08 MaxDP=7.52D-07 DE=-9.60D-11 OVMax= 1.56D-06

Cycle 13 Pass 1 IDiag 1:

RMSU= 8.31D-09 CP: 9.99D-01 1.08D+00 4.79D-01 8.29D-01 7.90D-01

CP: 1.19D+00 1.06D+00 1.29D+00 1.04D+00 1.14D+00

CP: 1.01D+00 9.74D-01

E= -1658.67544495900 Delta-E= -0.000000000014 Rises=F Damp=F

DIIS: error= 6.20D-08 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1658.67544495900 IErMin=13 ErrMin= 6.20D-08

ErrMax= 6.20D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.39D-12 BMatP= 2.51D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.230D-05-0.458D-04-0.159D-04 0.565D-04 0.455D-03 0.283D-02

Coeff-Com: 0.223D-02-0.437D-02-0.147D-01-0.496D-01-0.253D-02 0.259D+00

Coeff-Com: 0.807D+00

Coeff: 0.230D-05-0.458D-04-0.159D-04 0.565D-04 0.455D-03 0.283D-02

Coeff: 0.223D-02-0.437D-02-0.147D-01-0.496D-01-0.253D-02 0.259D+00

Coeff: 0.807D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.30D-09 MaxDP=2.48D-07 DE=-1.41D-11 OVMax= 6.72D-07

Error on total polarization charges = 0.04168

SCF Done: E(UB3LYP) = -1658.67544496 A.U. after 13 cycles

NFock= 13 Conv=0.63D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7554 S= 0.5027

<L.S>= 0.000000000000E+00

KE= 1.655171799933D+03 PE=-6.142151605566D+03 EE= 1.728562590495D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.62

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7554, after 0.7500

Leave Link 502 at Sat Aug 17 17:56:51 2019, MaxMem= 1342177280 cpu: 335.4

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 338

Leave Link 701 at Sat Aug 17 17:56:52 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:56:52 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:56:55 2019, MaxMem= 1342177280 cpu: 38.3

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.51988252D+00-3.00556969D+00 5.72426301D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.003276522 0.004583666 -0.004138303

2 6 0.001987722 0.004995772 0.003061716

3 8 0.000536982 -0.001106607 -0.000579524

4 8 -0.001525769 -0.006423625 -0.003358610

5 6 0.002966464 0.006272551 -0.000278538

6 16 -0.000672018 -0.001228304 0.003467347

7 6 0.002024199 0.000809155 0.001500152

8 16 -0.004484443 -0.000594086 0.000144971

9 16 0.000478580 -0.004150085 -0.002007745

10 6 -0.000803507 0.002676875 -0.002476581

11 6 -0.000048567 0.002175198 0.002369939

12 6 -0.001340191 0.000525865 -0.000737693

13 6 0.000515276 -0.001380251 0.001728679

14 1 0.003470785 -0.003962913 0.002339162

15 1 -0.000345724 -0.001076463 0.002500564

16 1 -0.002348272 -0.002094600 -0.000244816

17 1 0.001576464 -0.000081581 -0.002030167

18 1 -0.001080641 0.000272741 -0.000362062

19 1 0.001718402 -0.000493003 0.000752845

20 1 0.001262987 -0.000583882 0.000540422

21 1 0.000392018 -0.000473158 -0.001750761

22 1 -0.001720152 0.001590379 0.001916903

23 1 0.000342350 -0.001731457 0.000924923

24 1 -0.000715244 0.000839116 -0.001819205

25 1 -0.000355806 -0.002122225 -0.000351219

26 1 0.000517539 0.001072781 -0.001307742

27 1 0.000927088 0.001688142 0.000195344

-------------------------------------------------------------------

Cartesian Forces: Max 0.006423625 RMS 0.002178868

Leave Link 716 at Sat Aug 17 17:56:55 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.007643134 RMS 0.001772167

Search for a local minimum.

Step number 58 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .17722D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43 45 44 47 46

49 48 51 50 53

54 55 56 52 58

57

DE= 1.57D-03 DEPred=-1.39D-05 R=-1.13D+02

Trust test=-1.13D+02 RLast= 6.99D-01 DXMaxT set to 5.98D-02

ITU= -1 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 1 1 1 -1

ITU= -1 0 -1 -1 -1 0 -1 0 0 -1 -1 0 0 -1 0 0 -1 1 -1 1

ITU= -1 1 1 -1 1 -1 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.99458.

Iteration 1 RMS(Cart)= 0.10559947 RMS(Int)= 0.00467557

Iteration 2 RMS(Cart)= 0.00915629 RMS(Int)= 0.00002962

Iteration 3 RMS(Cart)= 0.00005180 RMS(Int)= 0.00000035

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000035

ITry= 1 IFail=0 DXMaxC= 4.29D-01 DCOld= 1.00D+10 DXMaxT= 5.98D-02 DXLimC= 3.00D+00 Rises=T

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.81190 0.00748 0.02391 0.00000 0.02391 2.83581

R2 2.29373 -0.00083 -0.00457 0.00000 -0.00457 2.28916

R3 2.53658 0.00764 0.01648 0.00000 0.01648 2.55306

R4 2.87839 -0.00423 -0.01326 0.00000 -0.01326 2.86513

R5 3.63893 -0.00374 -0.02776 0.00000 -0.02776 3.61117

R6 2.06765 -0.00363 -0.00952 0.00000 -0.00952 2.05813

R7 1.83914 -0.00082 -0.00222 0.00000 -0.00222 1.83692

R8 2.07094 -0.00293 -0.00960 0.00000 -0.00960 2.06133

R9 2.07550 -0.00255 -0.00683 0.00000 -0.00683 2.06867

R10 2.06056 -0.00038 -0.00052 0.00000 -0.00052 2.06004

R11 3.31546 -0.00131 -0.00060 0.00000 -0.00060 3.31487

R12 3.41283 -0.00487 -0.02493 0.00000 -0.02493 3.38790

R13 3.26922 -0.00454 -0.01534 0.00000 -0.01534 3.25388

R14 3.45922 0.00239 0.01309 0.00000 0.01309 3.47230

R15 2.88888 -0.00254 -0.00747 0.00000 -0.00747 2.88141

R16 2.06738 -0.00090 -0.00311 0.00000 -0.00311 2.06428

R17 2.06029 0.00014 -0.00024 0.00000 -0.00024 2.06005

R18 2.90058 -0.00078 -0.00644 0.00000 -0.00644 2.89414

R19 2.07518 -0.00105 -0.00298 0.00000 -0.00298 2.07220

R20 2.07666 -0.00248 -0.00548 0.00000 -0.00548 2.07118

R21 2.88252 0.00169 0.00367 0.00000 0.00367 2.88620

R22 2.07768 -0.00189 -0.00576 0.00000 -0.00576 2.07192

R23 2.07509 -0.00133 -0.00327 0.00000 -0.00327 2.07182

R24 2.07150 -0.00142 -0.00384 0.00000 -0.00384 2.06766

R25 2.07453 -0.00167 -0.00528 0.00000 -0.00528 2.06925

R26 2.07176 -0.00104 -0.00267 0.00000 -0.00267 2.06909

A1 2.17375 0.00070 0.00250 0.00000 0.00250 2.17625

A2 1.97905 0.00037 -0.00148 0.00000 -0.00148 1.97757

A3 2.12954 -0.00104 -0.00075 0.00000 -0.00075 2.12879

A4 2.01814 0.00136 0.00935 0.00000 0.00935 2.02749

A5 1.84321 -0.00064 -0.01381 0.00000 -0.01381 1.82941

A6 1.84310 0.00236 0.03022 0.00000 0.03022 1.87332

A7 1.96059 -0.00154 -0.01411 0.00000 -0.01411 1.94648

A8 1.96698 -0.00266 -0.02562 0.00000 -0.02562 1.94136

A9 1.81508 0.00142 0.01720 0.00000 0.01720 1.83228

A10 1.86542 0.00234 0.00702 0.00000 0.00702 1.87244

A11 1.89814 0.00211 0.01474 0.00000 0.01474 1.91288

A12 1.92742 -0.00014 -0.00096 0.00000 -0.00096 1.92646

A13 1.95830 -0.00145 -0.00605 0.00000 -0.00604 1.95225

A14 1.88527 -0.00057 -0.00177 0.00000 -0.00177 1.88350

A15 1.89020 -0.00003 0.00393 0.00000 0.00393 1.89414

A16 1.90275 0.00012 -0.00975 0.00000 -0.00975 1.89300

A17 1.79788 -0.00034 0.00083 0.00000 0.00083 1.79871

A18 1.96267 0.00035 0.00753 0.00000 0.00753 1.97020

A19 2.14371 0.00130 -0.00078 0.00000 -0.00078 2.14293

A20 2.15994 -0.00163 -0.00482 0.00000 -0.00482 2.15511

A21 1.80746 -0.00397 -0.01164 0.00000 -0.01164 1.79582

A22 1.94235 -0.00337 -0.01559 0.00000 -0.01559 1.92676

A23 1.86755 0.00222 0.01154 0.00000 0.01154 1.87909

A24 1.88132 0.00205 0.01054 0.00000 0.01054 1.89186

A25 1.94581 -0.00046 -0.00649 0.00000 -0.00649 1.93933

A26 1.94447 -0.00052 -0.00632 0.00000 -0.00632 1.93815

A27 1.87879 0.00038 0.00797 0.00000 0.00797 1.88676

A28 1.93577 0.00264 0.01708 0.00000 0.01708 1.95285

A29 1.90936 -0.00024 0.00668 0.00000 0.00668 1.91604

A30 1.93549 -0.00194 -0.01818 0.00000 -0.01818 1.91731

A31 1.89955 -0.00051 0.00733 0.00000 0.00733 1.90687

A32 1.91100 -0.00008 -0.00257 0.00000 -0.00257 1.90843

A33 1.87122 0.00005 -0.01123 0.00000 -0.01123 1.85999

A34 1.97097 -0.00028 -0.00488 0.00000 -0.00488 1.96609

A35 1.90585 0.00053 0.00033 0.00000 0.00033 1.90618

A36 1.90354 -0.00041 0.00425 0.00000 0.00425 1.90779

A37 1.91887 -0.00030 -0.00601 0.00000 -0.00601 1.91286

A38 1.90116 0.00078 0.01160 0.00000 0.01160 1.91276

A39 1.86011 -0.00033 -0.00528 0.00000 -0.00528 1.85482

A40 1.93199 0.00206 0.01349 0.00000 0.01349 1.94549

A41 1.93548 0.00061 0.00653 0.00000 0.00653 1.94201

A42 1.94838 -0.00046 -0.00553 0.00000 -0.00553 1.94286

A43 1.88271 -0.00119 -0.00571 0.00000 -0.00571 1.87700

A44 1.89273 -0.00138 -0.01551 0.00000 -0.01551 1.87722

A45 1.87003 0.00023 0.00586 0.00000 0.00586 1.87588

D1 2.58059 0.00024 0.13420 0.00000 0.13420 2.71479

D2 -1.52330 -0.00134 0.11147 0.00000 0.11147 -1.41183

D3 0.39307 0.00092 0.13705 0.00000 0.13705 0.53013

D4 -0.60466 0.00086 0.14195 0.00000 0.14195 -0.46271

D5 1.57464 -0.00073 0.11922 0.00000 0.11922 1.69386

D6 -2.79218 0.00153 0.14480 0.00000 0.14480 -2.64738

D7 -3.00495 -0.00233 -0.09479 0.00000 -0.09479 -3.09975

D8 0.09423 -0.00169 -0.08719 0.00000 -0.08719 0.00704

D9 -3.10039 -0.00117 -0.04346 0.00000 -0.04346 3.13934

D10 -1.03451 -0.00067 -0.03717 0.00000 -0.03717 -1.07168

D11 1.09215 -0.00162 -0.05441 0.00000 -0.05441 1.03774

D12 1.06547 -0.00010 -0.02064 0.00000 -0.02064 1.04483

D13 3.13135 0.00040 -0.01435 0.00000 -0.01435 3.11700

D14 -1.02518 -0.00056 -0.03158 0.00000 -0.03158 -1.05676

D15 -0.97800 0.00092 -0.01626 0.00000 -0.01626 -0.99426

D16 1.08787 0.00142 -0.00997 0.00000 -0.00997 1.07790

D17 -3.06865 0.00047 -0.02721 0.00000 -0.02720 -3.09586

D18 -3.11785 0.00087 0.03010 0.00000 0.03010 -3.08775

D19 -0.90315 0.00111 0.02307 0.00000 0.02307 -0.88008

D20 1.22903 -0.00205 -0.00483 0.00000 -0.00482 1.22421

D21 1.80943 -0.00029 0.01304 0.00000 0.01304 1.82248

D22 -1.14237 -0.00024 0.00241 0.00000 0.00241 -1.13997

D23 2.62698 -0.00004 -0.03432 0.00000 -0.03432 2.59266

D24 -0.70646 0.00029 -0.02307 0.00000 -0.02307 -0.72953

D25 -3.05740 0.00000 0.02543 0.00000 0.02543 -3.03197

D26 -0.92773 -0.00116 0.01546 0.00000 0.01546 -0.91227

D27 1.08873 0.00140 0.03610 0.00000 0.03610 1.12482

D28 -3.00078 -0.00029 -0.12322 0.00000 -0.12322 -3.12399

D29 -0.90526 0.00058 -0.09851 0.00000 -0.09851 -1.00377

D30 1.15510 -0.00067 -0.11899 0.00000 -0.11899 1.03612

D31 1.19877 -0.00053 -0.12316 0.00000 -0.12315 1.07561

D32 -2.98891 0.00034 -0.09844 0.00000 -0.09844 -3.08735

D33 -0.92854 -0.00091 -0.11893 0.00000 -0.11893 -1.04746

D34 -0.90058 -0.00034 -0.12459 0.00000 -0.12459 -1.02517

D35 1.19493 0.00053 -0.09988 0.00000 -0.09988 1.09505

D36 -3.02789 -0.00072 -0.12036 0.00000 -0.12036 3.13494

D37 -3.02982 0.00047 -0.10248 0.00000 -0.10248 -3.13229

D38 -0.88926 0.00027 -0.11324 0.00000 -0.11324 -1.00250

D39 1.13708 -0.00006 -0.11700 0.00000 -0.11700 1.02007

D40 1.15202 -0.00055 -0.12662 0.00000 -0.12662 1.02539

D41 -2.99061 -0.00075 -0.13738 0.00000 -0.13738 -3.12800

D42 -0.96427 -0.00107 -0.14115 0.00000 -0.14115 -1.10542

D43 -0.88826 -0.00027 -0.11586 0.00000 -0.11586 -1.00412

D44 1.25229 -0.00047 -0.12662 0.00000 -0.12662 1.12568

D45 -3.00455 -0.00079 -0.13038 0.00000 -0.13038 -3.13494

D46 3.05326 0.00012 0.08260 0.00000 0.08260 3.13586

D47 -1.14088 0.00038 0.08873 0.00000 0.08873 -1.05215

D48 0.94300 0.00077 0.09684 0.00000 0.09684 1.03984

D49 0.91999 -0.00014 0.08985 0.00000 0.08985 1.00984

D50 3.00903 0.00011 0.09599 0.00000 0.09599 3.10502

D51 -1.19028 0.00050 0.10409 0.00000 0.10409 -1.08618

D52 -1.11228 -0.00003 0.09297 0.00000 0.09297 -1.01931

D53 0.97676 0.00022 0.09910 0.00000 0.09910 1.07587

D54 3.06063 0.00061 0.10721 0.00000 0.10721 -3.11534

Item Value Threshold Converged?

Maximum Force 0.007643 0.000450 NO

RMS Force 0.001772 0.000300 NO

Maximum Displacement 0.429011 0.001800 NO

RMS Displacement 0.104157 0.001200 NO

Predicted change in Energy=-5.986947D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:56:55 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.095609 -0.405616 -0.204715

2 6 0 -2.845050 0.073874 0.472134

3 8 0 -4.890484 0.310961 -0.772260

4 8 0 -4.244190 -1.747836 -0.164450

5 6 0 -2.299199 -0.812886 1.574157

6 16 0 -1.578478 0.295509 -0.941511

7 6 0 -0.116631 0.766008 -0.093757

8 16 0 1.082593 -0.561969 0.017920

9 16 0 0.022188 2.246662 0.774145

10 6 0 2.687671 0.332205 -0.003376

11 6 0 3.846119 -0.656924 -0.070989

12 6 0 5.203523 0.052271 -0.065469

13 6 0 6.376651 -0.922400 -0.145836

14 1 0 -3.039357 1.081620 0.836643

15 1 0 -5.054136 -1.963627 -0.656703

16 1 0 -1.393821 -0.366907 1.987994

17 1 0 -3.029109 -0.906792 2.384568

18 1 0 -2.057927 -1.811463 1.209461

19 1 0 2.685828 0.995974 -0.870945

20 1 0 2.750417 0.947885 0.894057

21 1 0 3.795119 -1.346876 0.779782

22 1 0 3.760215 -1.269488 -0.975778

23 1 0 5.248452 0.752133 -0.908263

24 1 0 5.291601 0.659474 0.843132

25 1 0 7.335642 -0.395596 -0.146400

26 1 0 6.379267 -1.611824 0.704876

27 1 0 6.330864 -1.526012 -1.058195

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.500644 0.000000

3 O 1.211369 2.405936 0.000000

4 O 1.351019 2.383581 2.241823 0.000000

5 C 2.560730 1.516163 3.671983 2.771258 0.000000

6 S 2.714847 1.910948 3.316364 3.447478 2.841930

7 C 4.149371 2.871158 4.843253 4.833337 3.168351

8 S 5.185343 4.004620 6.088023 5.460234 3.731132

9 S 4.994896 3.610162 5.502058 5.919371 3.922969

10 C 6.826258 5.559123 7.617090 7.239006 5.354318

11 C 7.946829 6.752836 8.817982 8.164063 6.363629

12 C 9.311440 8.066537 10.122028 9.618184 7.728371

13 C 10.485169 9.295925 11.351736 10.652885 8.845380

14 H 2.100468 1.089116 2.570827 3.234135 2.163542

15 H 1.884268 3.210256 2.283394 0.972055 3.727011

16 H 3.479817 2.144338 4.506124 3.829436 1.090811

17 H 2.844817 2.157078 3.861761 2.946399 1.094693

18 H 2.851043 2.172028 4.056510 2.582910 1.090124

19 H 6.956738 5.765825 7.607856 7.486840 5.839606

20 H 7.064513 5.679011 7.846378 7.570461 5.390870

21 H 8.007421 6.797427 8.977580 8.104494 6.169026

22 H 7.940704 6.894244 8.796239 8.059626 6.589928

23 H 9.441760 8.238343 10.149440 9.844458 8.098069

24 H 9.505373 8.166129 10.315319 9.886439 7.766756

25 H 11.431404 10.210263 12.262507 11.658533 9.796153

26 H 10.583257 9.379967 11.527633 10.659835 8.758409

27 H 10.521171 9.439223 11.374307 10.615072 9.050735

6 7 8 9 10

6 S 0.000000

7 C 1.754152 0.000000

8 S 2.955854 1.792800 0.000000

9 S 3.051656 1.721877 3.095923 0.000000

10 C 4.368234 2.839096 1.837465 3.372608 0.000000

11 C 5.575947 4.210540 2.766587 4.875193 1.524778

12 C 6.842671 5.367892 4.167291 5.689160 2.532140

13 C 8.087056 6.709408 5.308840 7.160204 3.899090

14 H 2.431866 3.083437 4.512445 3.276322 5.836618

15 H 4.155119 5.669812 6.330813 6.748549 8.101435

16 H 3.009135 2.692285 3.170467 3.210802 4.594876

17 H 3.822651 4.174072 4.756681 4.674200 6.318146

18 H 3.048915 3.479995 3.583834 4.580912 5.346680

19 H 4.322029 2.917307 2.405750 3.371278 1.092368

20 H 4.747024 3.037898 2.414314 3.023977 1.090131

21 H 5.876718 4.530909 2.924775 5.210427 2.158492

22 H 5.563455 4.466670 2.942394 5.422028 2.159012

23 H 6.842264 5.426576 4.465318 5.690162 2.748228

24 H 7.107419 5.489817 4.459670 5.503694 2.757560

25 H 8.976155 7.542445 6.257421 7.830424 4.706781

26 H 8.347108 6.963376 5.443241 7.436745 4.231874

27 H 8.117218 6.910404 5.443506 7.575614 4.223561

11 12 13 14 15

11 C 0.000000

12 C 1.531514 0.000000

13 C 2.545520 1.527309 0.000000

14 H 7.159338 8.355743 9.676909 0.000000

15 H 9.014714 10.470577 11.489475 3.944990 0.000000

16 H 5.637419 6.922237 8.077254 2.476213 4.789764

17 H 7.304859 8.642842 9.740201 2.519912 3.803546

18 H 6.150632 7.604447 8.588910 3.077682 3.533127

19 H 2.172160 2.806805 4.222336 5.975026 8.289281

20 H 2.169628 2.782183 4.210572 5.791604 8.473064

21 H 1.096561 2.157699 2.775114 7.253336 8.986277

22 H 1.096019 2.158437 2.766769 7.419351 8.847396

23 H 2.157082 1.096415 2.158284 8.475909 10.657483

24 H 2.158226 1.096362 2.158174 8.341650 10.777961

25 H 3.500107 2.180153 1.094160 10.525643 12.499029

26 H 2.816139 2.178307 1.094999 9.797066 11.519565

27 H 2.811378 2.178848 1.094917 9.909147 11.400479

16 17 18 19 20

16 H 0.000000

17 H 1.767177 0.000000

18 H 1.770280 1.772710 0.000000

19 H 5.164737 6.846852 5.891774 0.000000

20 H 4.483312 6.250150 5.552806 1.766837 0.000000

21 H 5.417121 7.024179 5.887156 3.073169 2.523962

22 H 6.013541 7.584088 6.238572 2.509506 3.071273

23 H 7.332144 9.061610 8.027450 2.574469 3.086559

24 H 6.859959 8.606012 7.762429 3.137092 2.558005

25 H 8.986656 10.681535 9.595946 4.907363 4.889967

26 H 7.976033 9.583109 8.454627 4.788039 4.444823

27 H 8.384124 9.992254 8.694570 4.436413 4.769806

21 22 23 24 25

21 H 0.000000

22 H 1.757611 0.000000

23 H 3.060639 2.511247 0.000000

24 H 2.503780 3.061776 1.754375 0.000000

25 H 3.781277 3.772961 2.500816 2.504087 0.000000

26 H 2.598775 3.130691 3.077216 2.522088 1.765937

27 H 3.136917 2.584730 2.526666 3.077574 1.766009

26 27

26 H 0.000000

27 H 1.765821 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 7.29D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.104516 -0.463653 -0.129431

2 6 0 -2.848631 0.118980 0.449553

3 8 0 -4.903506 0.150693 -0.801449

4 8 0 -4.253214 -1.780586 0.132924

5 6 0 -2.294598 -0.574613 1.678669

6 16 0 -1.592906 0.102265 -0.990793

7 6 0 -0.124427 0.703901 -0.243362

8 16 0 1.075195 -0.589336 0.076912

9 16 0 0.021543 2.307264 0.367196

10 6 0 2.680348 0.286514 -0.103769

11 6 0 3.837925 -0.702047 -0.015938

12 6 0 5.195558 -0.003820 -0.137774

13 6 0 6.367720 -0.980250 -0.065018

14 1 0 -3.039804 1.173372 0.644197

15 1 0 -5.066994 -2.073372 -0.310843

16 1 0 -1.385918 -0.067889 2.006388

17 1 0 -3.018278 -0.532327 2.498944

18 1 0 -2.056461 -1.620066 1.481973

19 1 0 2.672040 0.798004 -1.068951

20 1 0 2.750198 1.041759 0.679245

21 1 0 3.793253 -1.242049 0.937397

22 1 0 3.744862 -1.455396 -0.806546

23 1 0 5.234223 0.547282 -1.084831

24 1 0 5.290823 0.744867 0.657463

25 1 0 7.326848 -0.462286 -0.159749

26 1 0 6.376664 -1.519827 0.887767

27 1 0 6.314718 -1.726083 -0.864873

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3049763 0.1933792 0.1808575

Leave Link 202 at Sat Aug 17 17:56:55 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.2929465582 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0549970955 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.2379494627 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2320

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.15D-11

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 96

GePol: Fraction of low-weight points (<1% of avg) = 4.14%

GePol: Cavity surface area = 309.220 Ang\*\*2

GePol: Cavity volume = 320.406 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057861360 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.2321633267 Hartrees.

Leave Link 301 at Sat Aug 17 17:56:55 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:56:55 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:56:55 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Lowest energy guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000075 -0.000004 -0.000005 Ang= -0.01 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999928 0.011956 0.000636 0.000860 Ang= 1.38 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 5.42D-03

Max alpha theta= 5.058 degrees.

Max beta theta= 5.157 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 17:56:56 2019, MaxMem= 1342177280 cpu: 4.5

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16147200.

Iteration 1 A\*A^-1 deviation from unit magnitude is 4.66D-15 for 2303.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.56D-15 for 955 43.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.33D-15 for 2303.

Iteration 1 A^-1\*A deviation from orthogonality is 1.09D-10 for 785 739.

Iteration 2 A\*A^-1 deviation from unit magnitude is 3.00D-15 for 381.

Iteration 2 A\*A^-1 deviation from orthogonality is 2.21D-15 for 873 814.

Iteration 2 A^-1\*A deviation from unit magnitude is 8.88D-16 for 96.

Iteration 2 A^-1\*A deviation from orthogonality is 4.55D-16 for 2094 521.

E= -1658.67701858558

DIIS: error= 6.43D-06 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67701858558 IErMin= 1 ErrMin= 6.43D-06

ErrMax= 6.43D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.11D-08 BMatP= 3.11D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 88.626 Goal= None Shift= 0.000

Gap= 88.624 Goal= None Shift= 0.000

RMSDP=3.51D-07 MaxDP=2.06D-05 OVMax= 2.94D-05

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.51D-07 CP: 1.00D+00

E= -1658.67701858763 Delta-E= -0.000000002045 Rises=F Damp=F

DIIS: error= 6.58D-06 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67701858763 IErMin= 1 ErrMin= 6.43D-06

ErrMax= 6.58D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.42D-08 BMatP= 3.11D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.515D+00 0.485D+00

Coeff: 0.515D+00 0.485D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.51D-07 MaxDP=1.77D-05 DE=-2.04D-09 OVMax= 2.20D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.87D-07 CP: 1.00D+00 5.26D-01

E= -1658.67701859285 Delta-E= -0.000000005219 Rises=F Damp=F

DIIS: error= 2.11D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67701859285 IErMin= 3 ErrMin= 2.11D-06

ErrMax= 2.11D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.12D-09 BMatP= 3.11D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.239D-01 0.274D+00 0.702D+00

Coeff: 0.239D-01 0.274D+00 0.702D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=9.96D-08 MaxDP=5.63D-06 DE=-5.22D-09 OVMax= 1.05D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 5.94D-08 CP: 1.00D+00 6.62D-01 6.60D-01

E= -1658.67701859354 Delta-E= -0.000000000693 Rises=F Damp=F

DIIS: error= 1.66D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67701859354 IErMin= 4 ErrMin= 1.66D-06

ErrMax= 1.66D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.21D-09 BMatP= 5.12D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.168D-01 0.151D+00 0.468D+00 0.398D+00

Coeff: -0.168D-01 0.151D+00 0.468D+00 0.398D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.89D-08 MaxDP=1.62D-06 DE=-6.93D-10 OVMax= 4.54D-06

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.16D-08 CP: 1.00D+00 6.62D-01 7.48D-01 4.41D-01

E= -1658.67701859375 Delta-E= -0.000000000208 Rises=F Damp=F

DIIS: error= 1.69D-07 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67701859375 IErMin= 5 ErrMin= 1.69D-07

ErrMax= 1.69D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.32D-11 BMatP= 1.21D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.980D-02 0.598D-01 0.195D+00 0.197D+00 0.558D+00

Coeff: -0.980D-02 0.598D-01 0.195D+00 0.197D+00 0.558D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.46D-09 MaxDP=3.86D-07 DE=-2.08D-10 OVMax= 4.81D-07

Error on total polarization charges = 0.04162

SCF Done: E(UB3LYP) = -1658.67701859 A.U. after 5 cycles

NFock= 5 Conv=0.65D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655235878781D+03 PE=-6.147229592762D+03 EE= 1.731084532061D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.63

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:57:09 2019, MaxMem= 1342177280 cpu: 151.5

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 335

Leave Link 701 at Sat Aug 17 17:57:10 2019, MaxMem= 1342177280 cpu: 10.5

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:57:10 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:57:14 2019, MaxMem= 1342177280 cpu: 38.5

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.40896843D+00-2.94710027D+00 6.33969719D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000088882 -0.000055904 0.000075163

2 6 -0.000034390 -0.000052607 -0.000006417

3 8 -0.000116317 0.000204798 -0.000044385

4 8 0.000099447 -0.000093130 0.000001900

5 6 -0.000018021 -0.000012439 0.000016970

6 16 -0.000030545 0.000046214 0.000025478

7 6 0.000040955 0.000042285 0.000036249

8 16 -0.000009426 -0.000010921 0.000001668

9 16 -0.000016068 -0.000054432 0.000061809

10 6 -0.000000596 0.000014292 0.000010107

11 6 -0.000016812 0.000007458 -0.000006020

12 6 -0.000003478 0.000023955 -0.000015252

13 6 -0.000000371 -0.000016951 -0.000004250

14 1 0.000033527 -0.000003313 0.000016234

15 1 -0.000017948 0.000046772 -0.000032280

16 1 -0.000012854 -0.000045137 -0.000000048

17 1 0.000017619 -0.000055470 -0.000023451

18 1 -0.000004356 -0.000041440 -0.000038414

19 1 0.000037198 0.000029522 0.000023322

20 1 -0.000022860 -0.000023909 0.000045102

21 1 -0.000004821 -0.000016592 -0.000037948

22 1 -0.000016510 0.000023516 -0.000025821

23 1 0.000003364 0.000030212 0.000015775

24 1 0.000001324 -0.000015735 0.000007446

25 1 -0.000002742 -0.000000743 -0.000009748

26 1 0.000004544 -0.000022835 -0.000049643

27 1 0.000001253 0.000052532 -0.000043543

-------------------------------------------------------------------

Cartesian Forces: Max 0.000204798 RMS 0.000042702

Leave Link 716 at Sat Aug 17 17:57:14 2019, MaxMem= 1342177280 cpu: 0.3

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000211988 RMS 0.000030176

Search for a local minimum.

Step number 59 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .30176D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43 45 44 47 46

49 48 51 50 53

54 55 56 52 57

59

ITU= 0 -1 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 1 1 1

ITU= -1 -1 0 -1 -1 -1 0 -1 0 0 -1 -1 0 0 -1 0 0 -1 1 -1

ITU= 1 -1 1 1 -1 1 -1 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Use linear search instead of GDIIS.

Eigenvalues --- 0.00004 0.00030 0.00045 0.00160 0.00260

Eigenvalues --- 0.00354 0.00515 0.00626 0.01368 0.01696

Eigenvalues --- 0.02600 0.02851 0.03482 0.03637 0.03998

Eigenvalues --- 0.04152 0.04640 0.04823 0.05044 0.05204

Eigenvalues --- 0.05377 0.05428 0.05620 0.05806 0.06569

Eigenvalues --- 0.08124 0.08307 0.09842 0.10570 0.11129

Eigenvalues --- 0.11995 0.12777 0.13841 0.14314 0.15683

Eigenvalues --- 0.15948 0.15995 0.16145 0.16668 0.17166

Eigenvalues --- 0.18904 0.19369 0.19898 0.21370 0.21694

Eigenvalues --- 0.22329 0.22765 0.24397 0.25029 0.25791

Eigenvalues --- 0.27015 0.28523 0.28979 0.29149 0.29534

Eigenvalues --- 0.30589 0.32073 0.33176 0.33539 0.33863

Eigenvalues --- 0.33900 0.33941 0.34000 0.34042 0.34091

Eigenvalues --- 0.34129 0.34186 0.34398 0.34585 0.35052

Eigenvalues --- 0.36184 0.38852 0.47222 0.52394 0.87209

RFO step: Lambda=-2.36775786D-06 EMin= 3.56385680D-05

Quartic linear search produced a step of -0.00186.

Iteration 1 RMS(Cart)= 0.02150195 RMS(Int)= 0.00021042

Iteration 2 RMS(Cart)= 0.00033839 RMS(Int)= 0.00000290

Iteration 3 RMS(Cart)= 0.00000010 RMS(Int)= 0.00000290

ITry= 1 IFail=0 DXMaxC= 1.20D-01 DCOld= 1.00D+10 DXMaxT= 5.98D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83581 -0.00007 0.00000 -0.00087 -0.00087 2.83494

R2 2.28916 0.00021 0.00000 -0.00085 -0.00085 2.28830

R3 2.55306 0.00008 0.00000 -0.00128 -0.00128 2.55178

R4 2.86513 -0.00001 0.00000 0.00083 0.00083 2.86596

R5 3.61117 -0.00002 0.00000 -0.00544 -0.00544 3.60573

R6 2.05813 0.00000 0.00000 -0.00099 -0.00099 2.05715

R7 1.83692 0.00001 0.00000 -0.00037 -0.00037 1.83655

R8 2.06133 -0.00001 0.00000 -0.00035 -0.00035 2.06099

R9 2.06867 -0.00002 0.00000 -0.00007 -0.00007 2.06860

R10 2.06004 0.00001 0.00000 -0.00027 -0.00027 2.05977

R11 3.31487 0.00000 0.00000 0.00260 0.00260 3.31747

R12 3.38790 -0.00002 0.00000 -0.00119 -0.00119 3.38672

R13 3.25388 -0.00004 0.00000 -0.00010 -0.00010 3.25377

R14 3.47230 0.00000 0.00000 -0.00159 -0.00159 3.47072

R15 2.88141 -0.00003 0.00000 -0.00004 -0.00004 2.88138

R16 2.06428 0.00001 0.00000 -0.00018 -0.00018 2.06410

R17 2.06005 0.00001 0.00000 -0.00018 -0.00018 2.05987

R18 2.89414 0.00001 0.00000 -0.00055 -0.00055 2.89359

R19 2.07220 0.00000 0.00000 -0.00018 -0.00018 2.07202

R20 2.07118 0.00000 0.00000 -0.00049 -0.00049 2.07069

R21 2.88620 0.00001 0.00000 -0.00035 -0.00035 2.88584

R22 2.07192 0.00001 0.00000 -0.00037 -0.00037 2.07156

R23 2.07182 -0.00001 0.00000 -0.00027 -0.00027 2.07155

R24 2.06766 0.00000 0.00000 -0.00028 -0.00028 2.06738

R25 2.06925 0.00000 0.00000 -0.00023 -0.00023 2.06902

R26 2.06909 -0.00001 0.00000 -0.00025 -0.00025 2.06884

A1 2.17625 -0.00002 0.00000 0.00136 0.00136 2.17760

A2 1.97757 -0.00009 0.00000 -0.00034 -0.00034 1.97723

A3 2.12879 0.00012 0.00000 -0.00090 -0.00090 2.12789

A4 2.02749 -0.00004 0.00000 -0.00238 -0.00238 2.02511

A5 1.82941 0.00002 0.00000 0.00507 0.00507 1.83448

A6 1.87332 0.00003 0.00000 0.00167 0.00167 1.87499

A7 1.94648 0.00003 0.00000 -0.00067 -0.00067 1.94581

A8 1.94136 0.00000 0.00000 -0.00135 -0.00135 1.94001

A9 1.83228 -0.00003 0.00000 -0.00199 -0.00199 1.83029

A10 1.87244 -0.00004 0.00000 -0.00131 -0.00131 1.87113

A11 1.91288 0.00000 0.00000 0.00074 0.00074 1.91362

A12 1.92646 0.00000 0.00000 -0.00020 -0.00020 1.92627

A13 1.95225 0.00000 0.00000 0.00021 0.00021 1.95246

A14 1.88350 0.00000 0.00000 -0.00071 -0.00071 1.88279

A15 1.89414 0.00001 0.00000 0.00038 0.00038 1.89452

A16 1.89300 0.00000 0.00000 -0.00046 -0.00046 1.89254

A17 1.79871 -0.00008 0.00000 -0.00246 -0.00246 1.79625

A18 1.97020 -0.00002 0.00000 -0.00214 -0.00216 1.96804

A19 2.14293 -0.00001 0.00000 0.00011 0.00009 2.14302

A20 2.15511 0.00002 0.00000 0.00029 0.00028 2.15539

A21 1.79582 0.00000 0.00000 -0.00050 -0.00050 1.79532

A22 1.92676 -0.00005 0.00000 -0.00186 -0.00186 1.92490

A23 1.87909 0.00005 0.00000 0.00188 0.00188 1.88097

A24 1.89186 -0.00001 0.00000 0.00048 0.00048 1.89234

A25 1.93933 -0.00002 0.00000 0.00191 0.00191 1.94124

A26 1.93815 0.00003 0.00000 -0.00193 -0.00193 1.93622

A27 1.88676 0.00000 0.00000 -0.00036 -0.00036 1.88640

A28 1.95285 0.00001 0.00000 0.00068 0.00068 1.95352

A29 1.91604 -0.00001 0.00000 -0.00121 -0.00121 1.91483

A30 1.91731 -0.00001 0.00000 0.00007 0.00007 1.91738

A31 1.90687 0.00000 0.00000 0.00055 0.00055 1.90743

A32 1.90843 0.00000 0.00000 -0.00069 -0.00069 1.90773

A33 1.85999 0.00000 0.00000 0.00060 0.00060 1.86059

A34 1.96609 -0.00001 0.00000 -0.00002 -0.00002 1.96606

A35 1.90618 0.00001 0.00000 -0.00054 -0.00054 1.90564

A36 1.90779 0.00000 0.00000 0.00031 0.00031 1.90810

A37 1.91286 0.00000 0.00000 0.00096 0.00096 1.91381

A38 1.91276 0.00001 0.00000 -0.00053 -0.00053 1.91223

A39 1.85482 0.00000 0.00000 -0.00019 -0.00019 1.85463

A40 1.94549 0.00000 0.00000 0.00012 0.00012 1.94561

A41 1.94201 0.00002 0.00000 -0.00001 -0.00001 1.94200

A42 1.94286 -0.00001 0.00000 0.00083 0.00083 1.94369

A43 1.87700 -0.00001 0.00000 -0.00080 -0.00080 1.87620

A44 1.87722 0.00000 0.00000 -0.00037 -0.00037 1.87685

A45 1.87588 0.00000 0.00000 0.00017 0.00017 1.87605

D1 2.71479 -0.00002 0.00000 -0.03571 -0.03571 2.67908

D2 -1.41183 0.00000 0.00000 -0.03422 -0.03422 -1.44605

D3 0.53013 -0.00002 0.00000 -0.03356 -0.03355 0.49657

D4 -0.46271 -0.00002 0.00000 -0.03196 -0.03196 -0.49467

D5 1.69386 0.00000 0.00000 -0.03047 -0.03047 1.66338

D6 -2.64738 -0.00002 0.00000 -0.02980 -0.02980 -2.67717

D7 -3.09975 -0.00001 0.00000 0.00175 0.00175 -3.09800

D8 0.00704 -0.00001 0.00000 0.00543 0.00543 0.01247

D9 3.13934 0.00000 0.00000 0.00987 0.00987 -3.13397

D10 -1.07168 0.00000 0.00000 0.00934 0.00934 -1.06234

D11 1.03774 0.00000 0.00000 0.00876 0.00876 1.04650

D12 1.04483 0.00000 0.00000 0.00538 0.00538 1.05022

D13 3.11700 -0.00001 0.00000 0.00484 0.00485 3.12185

D14 -1.05676 -0.00001 0.00000 0.00427 0.00427 -1.05249

D15 -0.99426 0.00001 0.00000 0.00915 0.00915 -0.98512

D16 1.07790 0.00001 0.00000 0.00861 0.00861 1.08652

D17 -3.09586 0.00000 0.00000 0.00803 0.00803 -3.08783

D18 -3.08775 0.00003 0.00000 -0.02151 -0.02151 -3.10926

D19 -0.88008 0.00001 0.00000 -0.02139 -0.02139 -0.90147

D20 1.22421 0.00001 0.00000 -0.02461 -0.02460 1.19960

D21 1.82248 -0.00003 0.00000 -0.00812 -0.00811 1.81436

D22 -1.13997 0.00003 0.00000 0.00219 0.00219 -1.13778

D23 2.59266 0.00005 0.00000 0.01442 0.01442 2.60707

D24 -0.72953 -0.00002 0.00000 0.00400 0.00400 -0.72553

D25 -3.03197 0.00000 0.00000 0.00750 0.00750 -3.02446

D26 -0.91227 -0.00002 0.00000 0.00991 0.00991 -0.90236

D27 1.12482 0.00000 0.00000 0.01074 0.01074 1.13556

D28 -3.12399 0.00001 0.00000 0.00884 0.00884 -3.11515

D29 -1.00377 0.00001 0.00000 0.00916 0.00916 -0.99461

D30 1.03612 0.00000 0.00000 0.00922 0.00922 1.04534

D31 1.07561 0.00000 0.00000 0.00648 0.00648 1.08209

D32 -3.08735 0.00000 0.00000 0.00680 0.00679 -3.08056

D33 -1.04746 -0.00001 0.00000 0.00685 0.00685 -1.04061

D34 -1.02517 -0.00001 0.00000 0.00695 0.00695 -1.01822

D35 1.09505 -0.00001 0.00000 0.00727 0.00727 1.10232

D36 3.13494 -0.00002 0.00000 0.00733 0.00733 -3.14092

D37 -3.13229 0.00000 0.00000 -0.00441 -0.00441 -3.13670

D38 -1.00250 0.00000 0.00000 -0.00359 -0.00359 -1.00609

D39 1.02007 0.00000 0.00000 -0.00394 -0.00394 1.01613

D40 1.02539 0.00000 0.00000 -0.00371 -0.00371 1.02168

D41 -3.12800 0.00000 0.00000 -0.00289 -0.00289 -3.13089

D42 -1.10542 0.00000 0.00000 -0.00324 -0.00324 -1.10867

D43 -1.00412 0.00000 0.00000 -0.00435 -0.00435 -1.00847

D44 1.12568 0.00000 0.00000 -0.00352 -0.00353 1.12215

D45 -3.13494 0.00000 0.00000 -0.00388 -0.00388 -3.13882

D46 3.13586 0.00001 0.00000 -0.00983 -0.00983 3.12603

D47 -1.05215 0.00001 0.00000 -0.01077 -0.01077 -1.06292

D48 1.03984 0.00002 0.00000 -0.01001 -0.01001 1.02983

D49 1.00984 0.00000 0.00000 -0.00981 -0.00981 1.00003

D50 3.10502 0.00000 0.00000 -0.01075 -0.01075 3.09427

D51 -1.08618 0.00001 0.00000 -0.00999 -0.00998 -1.09617

D52 -1.01931 0.00000 0.00000 -0.00982 -0.00982 -1.02913

D53 1.07587 0.00000 0.00000 -0.01077 -0.01077 1.06510

D54 -3.11534 0.00001 0.00000 -0.01000 -0.01000 -3.12534

Item Value Threshold Converged?

Maximum Force 0.000212 0.000450 YES

RMS Force 0.000030 0.000300 YES

Maximum Displacement 0.119959 0.001800 NO

RMS Displacement 0.021549 0.001200 NO

Predicted change in Energy=-1.063408D-06

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:57:14 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.101089 -0.397776 -0.183852

2 6 0 -2.834566 0.067413 0.471947

3 8 0 -4.914413 0.329737 -0.708780

4 8 0 -4.245425 -1.740345 -0.173947

5 6 0 -2.284158 -0.827114 1.565998

6 16 0 -1.584320 0.277574 -0.954045

7 6 0 -0.118140 0.766692 -0.121603

8 16 0 1.081090 -0.558872 0.007275

9 16 0 0.017479 2.256892 0.730209

10 6 0 2.684385 0.336799 -0.012958

11 6 0 3.842274 -0.653185 -0.077074

12 6 0 5.200543 0.053494 -0.058204

13 6 0 6.372501 -0.923051 -0.128715

14 1 0 -3.009930 1.076534 0.840677

15 1 0 -5.066704 -1.944755 -0.651676

16 1 0 -1.372311 -0.389091 1.973601

17 1 0 -3.007110 -0.918849 2.382819

18 1 0 -2.053571 -1.826101 1.195973

19 1 0 2.684007 1.001526 -0.879676

20 1 0 2.746854 0.951640 0.884952

21 1 0 3.783110 -1.346839 0.770028

22 1 0 3.762633 -1.260784 -0.985464

23 1 0 5.253630 0.754496 -0.899321

24 1 0 5.281736 0.659229 0.851844

25 1 0 7.332103 -0.397674 -0.129819

26 1 0 6.372212 -1.606242 0.726860

27 1 0 6.329340 -1.532988 -1.036827

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.500184 0.000000

3 O 1.210918 2.405970 0.000000

4 O 1.350341 2.382370 2.240275 0.000000

5 C 2.558817 1.516601 3.664855 2.776323 0.000000

6 S 2.717245 1.908071 3.339520 3.429581 2.839142

7 C 4.150149 2.867100 4.851797 4.829332 3.174878

8 S 5.188203 3.992557 6.103148 5.458981 3.718395

9 S 4.984513 3.604814 5.487092 5.913354 3.937915

10 C 6.827258 5.546758 7.630593 7.236208 5.341742

11 C 7.948185 6.738018 8.834295 8.161016 6.345322

12 C 9.313419 8.052592 10.139620 9.615485 7.709361

13 C 10.486899 9.279650 11.371033 10.649430 8.821508

14 H 2.100922 1.088595 2.566238 3.238937 2.162571

15 H 1.882663 3.208394 2.280300 0.971859 3.729580

16 H 3.478635 2.145123 4.500930 3.833097 1.090627

17 H 2.838328 2.157294 3.841192 2.957251 1.094656

18 H 2.852431 2.172456 4.057110 2.586167 1.089983

19 H 6.962739 5.757960 7.629973 7.485515 5.831630

20 H 7.060990 5.666100 7.849953 7.567035 5.379486

21 H 7.998200 6.773670 8.980239 8.093411 6.141288

22 H 7.951445 6.885578 8.825952 8.063344 6.577363

23 H 9.452534 8.232338 10.178695 9.847966 8.086874

24 H 9.498806 8.146713 10.320153 9.878107 7.743512

25 H 11.433319 10.195077 12.281754 11.655207 9.774082

26 H 10.582051 9.361136 11.541100 10.656624 8.731777

27 H 10.526638 9.424163 11.401725 10.611937 9.025813

6 7 8 9 10

6 S 0.000000

7 C 1.755529 0.000000

8 S 2.954351 1.792173 0.000000

9 S 3.052896 1.721822 3.095550 0.000000

10 C 4.371613 2.837386 1.836625 3.369190 0.000000

11 C 5.575242 4.207483 2.764082 4.873326 1.524758

12 C 6.847416 5.366662 4.165234 5.686889 2.532461

13 C 8.089109 6.706990 5.305672 7.157939 3.899080

14 H 2.427288 3.063402 4.483921 3.251254 5.805266

15 H 4.142122 5.667558 6.336423 6.738870 8.105112

16 H 3.010067 2.701604 3.148720 3.237093 4.574945

17 H 3.819741 4.178436 4.741958 4.686639 6.301548

18 H 3.044376 3.493491 3.583988 4.601849 5.346763

19 H 4.329925 2.912362 2.406422 3.358280 1.092274

20 H 4.753457 3.042294 2.413863 3.029375 1.090034

21 H 5.866895 4.525680 2.916093 5.212336 2.157523

22 H 5.563941 4.462882 2.944297 5.416987 2.158855

23 H 6.854781 5.427791 4.467320 5.685933 2.749751

24 H 7.109826 5.487970 4.454492 5.502701 2.756461

25 H 8.979862 7.540686 6.254594 7.828799 4.706845

26 H 8.347492 6.962426 5.441577 7.436831 4.233534

27 H 8.118559 6.906241 5.439042 7.571340 4.222571

11 12 13 14 15

11 C 0.000000

12 C 1.531223 0.000000

13 C 2.545102 1.527121 0.000000

14 H 7.126492 8.322647 9.641995 0.000000

15 H 9.020434 10.476716 11.496643 3.947864 0.000000

16 H 5.609538 6.893948 8.042821 2.472522 4.791734

17 H 7.282562 8.617981 9.710043 2.521857 3.808225

18 H 6.144702 7.597894 8.577236 3.076710 3.536504

19 H 2.173436 2.811856 4.227639 5.948626 8.294943

20 H 2.168156 2.777912 4.205628 5.758309 8.473608

21 H 1.096467 2.157781 2.773496 7.212705 8.983205

22 H 1.095761 2.157480 2.767579 7.393608 8.862078

23 H 2.156289 1.096221 2.158674 8.450901 10.670360

24 H 2.158093 1.096218 2.157516 8.302168 10.776434

25 H 3.499567 2.179961 1.094010 10.491558 12.505847

26 H 2.820499 2.178040 1.094878 9.758833 11.526654

27 H 2.807254 2.179177 1.094785 9.877073 11.409983

16 17 18 19 20

16 H 0.000000

17 H 1.766541 0.000000

18 H 1.770259 1.772272 0.000000

19 H 5.150604 6.835241 5.894781 0.000000

20 H 4.466569 6.233012 5.554877 1.766452 0.000000

21 H 5.379985 6.992236 5.871794 3.073170 2.523894

22 H 5.990289 7.569126 6.237505 2.508520 3.070029

23 H 7.311947 9.045018 8.027760 2.581545 3.083249

24 H 6.828884 8.575499 7.752549 3.140625 2.551906

25 H 8.954958 10.652901 9.585875 4.911705 4.886197

26 H 7.938102 9.549156 8.441695 4.794192 4.439705

27 H 8.347850 9.961949 8.680121 4.442624 4.764537

21 22 23 24 25

21 H 0.000000

22 H 1.757719 0.000000

23 H 3.060191 2.508355 0.000000

24 H 2.505371 3.061017 1.753980 0.000000

25 H 3.782326 3.770703 2.497935 2.506933 0.000000

26 H 2.602422 3.140270 3.077138 2.517364 1.765199

27 H 3.127724 2.581611 2.531530 3.077396 1.765541

26 27

26 H 0.000000

27 H 1.765728 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 2.69D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.106871 -0.451930 -0.116266

2 6 0 -2.835807 0.102840 0.455729

3 8 0 -4.923801 0.191843 -0.736349

4 8 0 -4.251175 -1.778463 0.090874

5 6 0 -2.277835 -0.622645 1.665034

6 16 0 -1.595495 0.100887 -0.994222

7 6 0 -0.123550 0.704953 -0.252358

8 16 0 1.076506 -0.588766 0.060756

9 16 0 0.018031 2.303562 0.371402

10 6 0 2.679649 0.292638 -0.101267

11 6 0 3.837035 -0.697290 -0.027862

12 6 0 5.195423 0.003129 -0.121879

13 6 0 6.366834 -0.974455 -0.056863

14 1 0 -3.008573 1.155219 0.674107

15 1 0 -5.075761 -2.049683 -0.346170

16 1 0 -1.363165 -0.130675 1.997919

17 1 0 -2.995096 -0.593179 2.491436

18 1 0 -2.049856 -1.665246 1.443514

19 1 0 2.673268 0.823464 -1.055859

20 1 0 2.748376 1.032118 0.696618

21 1 0 3.783738 -1.259539 0.911965

22 1 0 3.751064 -1.431121 -0.837054

23 1 0 5.242685 0.573528 -1.056819

24 1 0 5.282958 0.735357 0.689215

25 1 0 7.326421 -0.455892 -0.141385

26 1 0 6.372470 -1.525176 0.889410

27 1 0 6.317343 -1.710596 -0.865689

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3124897 0.1934654 0.1807955

Leave Link 202 at Sat Aug 17 17:57:14 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.6186482720 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0550295137 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.5636187583 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2317

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.33D-11

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 79

GePol: Fraction of low-weight points (<1% of avg) = 3.41%

GePol: Cavity surface area = 309.298 Ang\*\*2

GePol: Cavity volume = 320.360 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0058114315 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.5578073268 Hartrees.

Leave Link 301 at Sat Aug 17 17:57:14 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:57:14 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:57:14 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999982 -0.006034 -0.000310 -0.000133 Ang= -0.69 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.63030635507

Leave Link 401 at Sat Aug 17 17:57:15 2019, MaxMem= 1342177280 cpu: 7.7

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16105467.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.11D-15 for 2292.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.66D-15 for 707 445.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.55D-15 for 2292.

Iteration 1 A^-1\*A deviation from orthogonality is 3.25D-12 for 1973 952.

E= -1658.67485173095

DIIS: error= 2.34D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67485173095 IErMin= 1 ErrMin= 2.34D-03

ErrMax= 2.34D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.31D-03 BMatP= 5.31D-03

IDIUse=3 WtCom= 9.77D-01 WtEn= 2.34D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.428 Goal= None Shift= 0.000

Gap= 0.484 Goal= None Shift= 0.000

GapD= 0.428 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=1.49D-04 MaxDP=5.23D-03 OVMax= 1.24D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.49D-04 CP: 1.00D+00

E= -1658.67701444901 Delta-E= -0.002162718059 Rises=F Damp=F

DIIS: error= 3.44D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67701444901 IErMin= 2 ErrMin= 3.44D-04

ErrMax= 3.44D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.09D-04 BMatP= 5.31D-03

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.44D-03

Coeff-Com: -0.634D-01 0.106D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.632D-01 0.106D+01

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.84D-05 MaxDP=1.48D-03 DE=-2.16D-03 OVMax= 2.03D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.68D-05 CP: 1.00D+00 1.06D+00

E= -1658.67702215855 Delta-E= -0.000007709544 Rises=F Damp=F

DIIS: error= 4.78D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67702215855 IErMin= 2 ErrMin= 3.44D-04

ErrMax= 4.78D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.29D-04 BMatP= 1.09D-04

IDIUse=3 WtCom= 3.14D-01 WtEn= 6.86D-01

Coeff-Com: -0.437D-01 0.595D+00 0.449D+00

Coeff-En: 0.000D+00 0.381D+00 0.619D+00

Coeff: -0.137D-01 0.448D+00 0.565D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.41D-05 MaxDP=1.39D-03 DE=-7.71D-06 OVMax= 2.39D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.33D-05 CP: 1.00D+00 1.08D+00 2.59D-01

E= -1658.67703139026 Delta-E= -0.000009231702 Rises=F Damp=F

DIIS: error= 3.98D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67703139026 IErMin= 2 ErrMin= 3.44D-04

ErrMax= 3.98D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.40D-05 BMatP= 1.09D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.98D-03

Coeff-Com: -0.116D-01 0.142D+00 0.425D+00 0.444D+00

Coeff-En: 0.000D+00 0.000D+00 0.413D+00 0.587D+00

Coeff: -0.116D-01 0.141D+00 0.425D+00 0.445D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.05D-05 MaxDP=5.50D-04 DE=-9.23D-06 OVMax= 1.08D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.00D-06 CP: 1.00D+00 1.08D+00 5.57D-01 5.40D-01

E= -1658.67704704117 Delta-E= -0.000015650912 Rises=F Damp=F

DIIS: error= 1.33D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67704704117 IErMin= 5 ErrMin= 1.33D-05

ErrMax= 1.33D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.98D-07 BMatP= 8.40D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.266D-02 0.256D-01 0.150D+00 0.178D+00 0.649D+00

Coeff: -0.266D-02 0.256D-01 0.150D+00 0.178D+00 0.649D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.73D-06 MaxDP=7.68D-05 DE=-1.57D-05 OVMax= 1.72D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.17D-06 CP: 1.00D+00 1.08D+00 5.94D-01 5.67D-01 7.53D-01

E= -1658.67704712499 Delta-E= -0.000000083824 Rises=F Damp=F

DIIS: error= 9.54D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67704712499 IErMin= 6 ErrMin= 9.54D-06

ErrMax= 9.54D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.95D-08 BMatP= 3.98D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.706D-03-0.142D-01 0.555D-02 0.192D-01 0.345D+00 0.644D+00

Coeff: 0.706D-03-0.142D-01 0.555D-02 0.192D-01 0.345D+00 0.644D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.24D-07 MaxDP=2.75D-05 DE=-8.38D-08 OVMax= 5.53D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 4.25D-07 CP: 1.00D+00 1.08D+00 5.92D-01 5.86D-01 8.56D-01

CP: 8.13D-01

E= -1658.67704714743 Delta-E= -0.000000022440 Rises=F Damp=F

DIIS: error= 1.77D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67704714743 IErMin= 7 ErrMin= 1.77D-06

ErrMax= 1.77D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.17D-09 BMatP= 8.95D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.521D-03-0.880D-02-0.668D-02-0.147D-02 0.131D+00 0.315D+00

Coeff-Com: 0.571D+00

Coeff: 0.521D-03-0.880D-02-0.668D-02-0.147D-02 0.131D+00 0.315D+00

Coeff: 0.571D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.67D-07 MaxDP=1.23D-05 DE=-2.24D-08 OVMax= 3.82D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.99D-07 CP: 1.00D+00 1.08D+00 5.95D-01 5.84D-01 8.85D-01

CP: 9.20D-01 8.68D-01

E= -1658.67704714933 Delta-E= -0.000000001898 Rises=F Damp=F

DIIS: error= 1.10D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67704714933 IErMin= 8 ErrMin= 1.10D-06

ErrMax= 1.10D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.72D-09 BMatP= 7.17D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.135D-03-0.177D-02-0.488D-02-0.480D-02 0.186D-02 0.350D-01

Coeff-Com: 0.325D+00 0.650D+00

Coeff: 0.135D-03-0.177D-02-0.488D-02-0.480D-02 0.186D-02 0.350D-01

Coeff: 0.325D+00 0.650D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.19D-07 MaxDP=5.94D-06 DE=-1.90D-09 OVMax= 1.39D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 7.18D-08 CP: 1.00D+00 1.08D+00 5.96D-01 5.87D-01 8.90D-01

CP: 9.62D-01 1.02D+00 8.74D-01

E= -1658.67704714987 Delta-E= -0.000000000536 Rises=F Damp=F

DIIS: error= 3.98D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67704714987 IErMin= 9 ErrMin= 3.98D-07

ErrMax= 3.98D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.76D-10 BMatP= 1.72D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.466D-04 0.116D-02-0.140D-02-0.266D-02-0.311D-01-0.577D-01

Coeff-Com: 0.686D-01 0.409D+00 0.614D+00

Coeff: -0.466D-04 0.116D-02-0.140D-02-0.266D-02-0.311D-01-0.577D-01

Coeff: 0.686D-01 0.409D+00 0.614D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=7.66D-08 MaxDP=3.71D-06 DE=-5.36D-10 OVMax= 9.88D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 2.88D-08 CP: 1.00D+00 1.08D+00 5.97D-01 5.87D-01 8.97D-01

CP: 9.89D-01 1.12D+00 1.07D+00 8.22D-01

E= -1658.67704715001 Delta-E= -0.000000000142 Rises=F Damp=F

DIIS: error= 1.32D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67704715001 IErMin=10 ErrMin= 1.32D-07

ErrMax= 1.32D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.56D-11 BMatP= 4.76D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.433D-04 0.842D-03 0.999D-04-0.517D-03-0.144D-01-0.336D-01

Coeff-Com: -0.216D-01 0.903D-01 0.274D+00 0.705D+00

Coeff: -0.433D-04 0.842D-03 0.999D-04-0.517D-03-0.144D-01-0.336D-01

Coeff: -0.216D-01 0.903D-01 0.274D+00 0.705D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.92D-08 MaxDP=1.49D-06 DE=-1.42D-10 OVMax= 3.47D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.17D-08 CP: 1.00D+00 1.08D+00 5.97D-01 5.88D-01 8.97D-01

CP: 1.00D+00 1.15D+00 1.12D+00 9.41D-01 8.48D-01

E= -1658.67704715004 Delta-E= -0.000000000030 Rises=F Damp=F

DIIS: error= 9.29D-08 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67704715004 IErMin=11 ErrMin= 9.29D-08

ErrMax= 9.29D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.18D-11 BMatP= 4.56D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.119D-04 0.175D-03 0.271D-03 0.208D-03-0.972D-03-0.544D-02

Coeff-Com: -0.237D-01-0.351D-01-0.642D-03 0.361D+00 0.704D+00

Coeff: -0.119D-04 0.175D-03 0.271D-03 0.208D-03-0.972D-03-0.544D-02

Coeff: -0.237D-01-0.351D-01-0.642D-03 0.361D+00 0.704D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.33D-08 MaxDP=6.76D-07 DE=-2.96D-11 OVMax= 1.75D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 4.68D-09 CP: 1.00D+00 1.08D+00 5.97D-01 5.88D-01 8.98D-01

CP: 1.01D+00 1.16D+00 1.16D+00 9.72D-01 1.01D+00

CP: 9.61D-01

E= -1658.67704715003 Delta-E= 0.000000000010 Rises=F Damp=F

DIIS: error= 3.62D-08 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=11 EnMin= -1658.67704715004 IErMin=12 ErrMin= 3.62D-08

ErrMax= 3.62D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.80D-12 BMatP= 1.18D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.133D-05-0.570D-04 0.116D-03 0.192D-03 0.203D-02 0.278D-02

Coeff-Com: -0.816D-02-0.333D-01-0.497D-01 0.750D-01 0.359D+00 0.652D+00

Coeff: 0.133D-05-0.570D-04 0.116D-03 0.192D-03 0.203D-02 0.278D-02

Coeff: -0.816D-02-0.333D-01-0.497D-01 0.750D-01 0.359D+00 0.652D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.86D-09 MaxDP=2.04D-07 DE= 1.00D-11 OVMax= 4.24D-07

Error on total polarization charges = 0.04161

SCF Done: E(UB3LYP) = -1658.67704715 A.U. after 12 cycles

NFock= 12 Conv=0.39D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655247735443D+03 PE=-6.147884725516D+03 EE= 1.731402135596D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.65

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:57:41 2019, MaxMem= 1342177280 cpu: 303.5

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 337

Leave Link 701 at Sat Aug 17 17:57:42 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:57:42 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:57:45 2019, MaxMem= 1342177280 cpu: 38.8

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.42219604D+00-2.96756702D+00 6.12871161D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000035452 0.000142317 0.000627342

2 6 0.000474248 -0.000271253 0.000274493

3 8 -0.000415810 0.000784284 -0.000587010

4 8 0.000340478 -0.000627425 -0.000140389

5 6 -0.000264006 -0.000029157 0.000167640

6 16 0.000335446 0.000179421 -0.000199423

7 6 -0.000364671 -0.000023211 0.000105916

8 16 0.000056066 -0.000037865 -0.000171954

9 16 -0.000039781 0.000028024 -0.000015396

10 6 0.000276075 -0.000125199 0.000238645

11 6 -0.000011424 0.000133871 -0.000044985

12 6 -0.000010135 0.000014556 0.000041108

13 6 0.000121012 0.000022423 0.000019215

14 1 -0.000302603 0.000217678 0.000055005

15 1 -0.000196784 -0.000204696 0.000043656

16 1 0.000098140 -0.000007610 -0.000068703

17 1 -0.000040340 -0.000033488 0.000044872

18 1 0.000064605 -0.000100918 -0.000119280

19 1 0.000029626 -0.000069379 -0.000110254

20 1 -0.000147389 0.000115490 0.000090357

21 1 0.000101050 -0.000079432 0.000018651

22 1 -0.000076924 -0.000141525 -0.000084312

23 1 0.000064143 0.000056965 -0.000127627

24 1 -0.000013271 0.000064722 0.000076798

25 1 0.000074535 0.000093166 -0.000012048

26 1 -0.000073623 -0.000109243 -0.000005680

27 1 -0.000043209 0.000007485 -0.000116637

-------------------------------------------------------------------

Cartesian Forces: Max 0.000784284 RMS 0.000209830

Leave Link 716 at Sat Aug 17 17:57:45 2019, MaxMem= 1342177280 cpu: 0.3

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.001005718 RMS 0.000174971

Search for a local minimum.

Step number 60 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .17497D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43 45 44 47 46

49 48 51 50 53

54 55 56 52 57

59 60

DE= -2.86D-05 DEPred=-1.06D-06 R= 2.69D+01

TightC=F SS= 1.41D+00 RLast= 1.04D-01 DXNew= 1.0064D-01 3.1195D-01

Trust test= 2.69D+01 RLast= 1.04D-01 DXMaxT set to 1.01D-01

ITU= 1 0 -1 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 1 1

ITU= 1 -1 -1 0 -1 -1 -1 0 -1 0 0 -1 -1 0 0 -1 0 0 -1 1

ITU= -1 1 -1 1 1 -1 1 -1 1 1 -1 0 0 -1 0 0 -1 -1 0 0

Eigenvalues --- 0.00021 0.00059 0.00105 0.00234 0.00251

Eigenvalues --- 0.00317 0.00361 0.00484 0.01546 0.01771

Eigenvalues --- 0.02496 0.03289 0.03534 0.03743 0.03999

Eigenvalues --- 0.04532 0.04804 0.04910 0.05108 0.05189

Eigenvalues --- 0.05375 0.05459 0.05596 0.05842 0.06995

Eigenvalues --- 0.08159 0.08308 0.10259 0.11164 0.11419

Eigenvalues --- 0.11945 0.12740 0.13788 0.14797 0.15210

Eigenvalues --- 0.15682 0.15977 0.16139 0.16603 0.17221

Eigenvalues --- 0.18031 0.19546 0.19982 0.20730 0.21920

Eigenvalues --- 0.22280 0.23299 0.24576 0.24980 0.27175

Eigenvalues --- 0.27505 0.28164 0.28779 0.29506 0.29978

Eigenvalues --- 0.30229 0.31385 0.33072 0.33455 0.33782

Eigenvalues --- 0.33872 0.33945 0.33982 0.34006 0.34044

Eigenvalues --- 0.34115 0.34162 0.34235 0.34411 0.34842

Eigenvalues --- 0.35040 0.36269 0.47473 0.52861 0.86773

En-DIIS/RFO-DIIS IScMMF= 0 using points: 60 59

RFO step: Lambda=-7.89119216D-06.

NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=F DC= 2.86D-05 SmlDif= 1.00D-05

RMS Error= 0.5020514575D-03 NUsed= 2 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.06757 0.93243

Iteration 1 RMS(Cart)= 0.02861609 RMS(Int)= 0.00024370

Iteration 2 RMS(Cart)= 0.00052891 RMS(Int)= 0.00000363

Iteration 3 RMS(Cart)= 0.00000014 RMS(Int)= 0.00000363

ITry= 1 IFail=0 DXMaxC= 9.95D-02 DCOld= 1.00D+10 DXMaxT= 1.01D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83494 0.00026 0.00081 -0.00339 -0.00258 2.83235

R2 2.28830 0.00101 0.00080 0.00047 0.00127 2.28957

R3 2.55178 0.00082 0.00119 -0.00020 0.00100 2.55277

R4 2.86596 0.00002 -0.00077 -0.00129 -0.00206 2.86390

R5 3.60573 0.00041 0.00507 0.00293 0.00800 3.61373

R6 2.05715 0.00027 0.00092 -0.00027 0.00065 2.05780

R7 1.83655 0.00018 0.00035 -0.00011 0.00024 1.83678

R8 2.06099 0.00006 0.00032 -0.00004 0.00028 2.06127

R9 2.06860 0.00006 0.00007 0.00010 0.00017 2.06877

R10 2.05977 0.00012 0.00025 -0.00019 0.00006 2.05983

R11 3.31747 -0.00012 -0.00242 -0.00149 -0.00392 3.31355

R12 3.38672 0.00033 0.00111 0.00274 0.00384 3.39056

R13 3.25377 0.00000 0.00010 0.00126 0.00135 3.25513

R14 3.47072 0.00021 0.00148 -0.00218 -0.00071 3.47001

R15 2.88138 0.00011 0.00004 -0.00001 0.00003 2.88140

R16 2.06410 0.00005 0.00017 -0.00040 -0.00023 2.06387

R17 2.05987 0.00012 0.00017 -0.00028 -0.00011 2.05976

R18 2.89359 0.00015 0.00051 0.00049 0.00100 2.89460

R19 2.07202 0.00007 0.00017 -0.00006 0.00011 2.07213

R20 2.07069 0.00015 0.00045 -0.00012 0.00034 2.07102

R21 2.88584 0.00008 0.00033 -0.00048 -0.00015 2.88570

R22 2.07156 0.00013 0.00034 0.00026 0.00060 2.07216

R23 2.07155 0.00010 0.00025 -0.00023 0.00002 2.07157

R24 2.06738 0.00011 0.00026 -0.00013 0.00013 2.06751

R25 2.06902 0.00008 0.00021 0.00010 0.00031 2.06933

R26 2.06884 0.00008 0.00023 -0.00037 -0.00014 2.06870

A1 2.17760 -0.00011 -0.00126 -0.00071 -0.00198 2.17562

A2 1.97723 -0.00033 0.00032 -0.00055 -0.00024 1.97699

A3 2.12789 0.00044 0.00084 0.00113 0.00196 2.12985

A4 2.02511 -0.00002 0.00221 0.00008 0.00229 2.02740

A5 1.83448 -0.00009 -0.00473 -0.00112 -0.00585 1.82863

A6 1.87499 -0.00012 -0.00155 -0.00150 -0.00306 1.87192

A7 1.94581 0.00012 0.00062 0.00050 0.00112 1.94694

A8 1.94001 0.00009 0.00126 0.00449 0.00576 1.94576

A9 1.83029 0.00002 0.00186 -0.00314 -0.00129 1.82900

A10 1.87113 0.00035 0.00122 -0.00100 0.00022 1.87136

A11 1.91362 -0.00007 -0.00069 -0.00117 -0.00186 1.91176

A12 1.92627 0.00004 0.00018 -0.00005 0.00013 1.92640

A13 1.95246 -0.00007 -0.00019 0.00045 0.00025 1.95271

A14 1.88279 0.00005 0.00066 -0.00027 0.00039 1.88318

A15 1.89452 0.00002 -0.00035 -0.00024 -0.00059 1.89393

A16 1.89254 0.00004 0.00043 0.00128 0.00171 1.89425

A17 1.79625 0.00045 0.00229 0.00095 0.00324 1.79950

A18 1.96804 0.00014 0.00201 -0.00155 0.00045 1.96850

A19 2.14302 -0.00014 -0.00009 0.00173 0.00163 2.14465

A20 2.15539 0.00006 -0.00026 0.00058 0.00031 2.15570

A21 1.79532 0.00029 0.00046 -0.00022 0.00025 1.79557

A22 1.92490 0.00031 0.00174 0.00089 0.00262 1.92752

A23 1.88097 -0.00014 -0.00175 -0.00129 -0.00304 1.87792

A24 1.89234 -0.00015 -0.00044 0.00035 -0.00010 1.89224

A25 1.94124 -0.00021 -0.00178 -0.00029 -0.00207 1.93917

A26 1.93622 0.00013 0.00180 0.00093 0.00273 1.93895

A27 1.88640 0.00005 0.00034 -0.00066 -0.00032 1.88608

A28 1.95352 -0.00007 -0.00063 -0.00146 -0.00209 1.95143

A29 1.91483 0.00010 0.00113 0.00042 0.00154 1.91637

A30 1.91738 -0.00001 -0.00007 0.00002 -0.00005 1.91733

A31 1.90743 -0.00003 -0.00052 -0.00029 -0.00081 1.90662

A32 1.90773 0.00006 0.00065 0.00071 0.00136 1.90909

A33 1.86059 -0.00004 -0.00056 0.00071 0.00015 1.86074

A34 1.96606 0.00001 0.00002 0.00008 0.00011 1.96617

A35 1.90564 0.00006 0.00050 -0.00039 0.00011 1.90576

A36 1.90810 -0.00004 -0.00029 0.00034 0.00005 1.90816

A37 1.91381 -0.00008 -0.00089 -0.00024 -0.00113 1.91268

A38 1.91223 0.00004 0.00049 -0.00013 0.00036 1.91260

A39 1.85463 0.00001 0.00018 0.00035 0.00052 1.85516

A40 1.94561 -0.00002 -0.00012 -0.00122 -0.00134 1.94427

A41 1.94200 -0.00001 0.00001 0.00011 0.00012 1.94212

A42 1.94369 -0.00008 -0.00078 0.00044 -0.00034 1.94335

A43 1.87620 0.00006 0.00075 0.00020 0.00095 1.87715

A44 1.87685 0.00004 0.00035 0.00109 0.00143 1.87828

A45 1.87605 0.00002 -0.00016 -0.00056 -0.00072 1.87533

D1 2.67908 0.00007 0.03330 -0.01261 0.02069 2.69976

D2 -1.44605 0.00014 0.03191 -0.01277 0.01913 -1.42692

D3 0.49657 0.00008 0.03128 -0.01742 0.01387 0.51045

D4 -0.49467 -0.00010 0.02980 -0.01733 0.01247 -0.48220

D5 1.66338 -0.00003 0.02841 -0.01749 0.01092 1.67431

D6 -2.67717 -0.00010 0.02778 -0.02213 0.00566 -2.67151

D7 -3.09800 -0.00003 -0.00163 0.00487 0.00325 -3.09475

D8 0.01247 -0.00021 -0.00506 0.00027 -0.00480 0.00767

D9 -3.13397 -0.00003 -0.00921 -0.00841 -0.01762 3.13159

D10 -1.06234 0.00002 -0.00871 -0.00950 -0.01821 -1.08056

D11 1.04650 0.00005 -0.00817 -0.00761 -0.01578 1.03072

D12 1.05022 0.00002 -0.00502 -0.00737 -0.01239 1.03783

D13 3.12185 0.00006 -0.00452 -0.00846 -0.01298 3.10887

D14 -1.05249 0.00009 -0.00398 -0.00657 -0.01055 -1.06305

D15 -0.98512 -0.00014 -0.00853 -0.00663 -0.01516 -1.00028

D16 1.08652 -0.00009 -0.00803 -0.00772 -0.01575 1.07076

D17 -3.08783 -0.00006 -0.00749 -0.00583 -0.01332 -3.10115

D18 -3.10926 -0.00004 0.02006 0.02075 0.04081 -3.06845

D19 -0.90147 -0.00006 0.01995 0.02038 0.04033 -0.86114

D20 1.19960 0.00012 0.02294 0.02414 0.04707 1.24667

D21 1.81436 0.00024 0.00757 -0.00615 0.00142 1.81578

D22 -1.13778 -0.00008 -0.00204 -0.01049 -0.01254 -1.15031

D23 2.60707 -0.00026 -0.01344 0.01131 -0.00213 2.60494

D24 -0.72553 0.00004 -0.00373 0.01582 0.01209 -0.71344

D25 -3.02446 0.00008 -0.00700 -0.00581 -0.01280 -3.03727

D26 -0.90236 -0.00007 -0.00924 -0.00644 -0.01568 -0.91804

D27 1.13556 -0.00017 -0.01001 -0.00773 -0.01774 1.11782

D28 -3.11515 -0.00009 -0.00824 0.00197 -0.00627 -3.12143

D29 -0.99461 -0.00011 -0.00854 0.00091 -0.00763 -1.00224

D30 1.04534 -0.00011 -0.00860 0.00203 -0.00657 1.03877

D31 1.08209 0.00002 -0.00604 0.00319 -0.00285 1.07924

D32 -3.08056 0.00000 -0.00634 0.00214 -0.00420 -3.08476

D33 -1.04061 -0.00001 -0.00639 0.00325 -0.00314 -1.04375

D34 -1.01822 0.00002 -0.00648 0.00359 -0.00288 -1.02110

D35 1.10232 -0.00001 -0.00678 0.00254 -0.00424 1.09808

D36 -3.14092 -0.00001 -0.00683 0.00365 -0.00318 3.13909

D37 -3.13670 0.00006 0.00411 0.00604 0.01015 -3.12655

D38 -1.00609 0.00000 0.00334 0.00551 0.00886 -0.99723

D39 1.01613 0.00003 0.00367 0.00590 0.00958 1.02571

D40 1.02168 0.00000 0.00346 0.00668 0.01014 1.03182

D41 -3.13089 -0.00005 0.00269 0.00615 0.00885 -3.12204

D42 -1.10867 -0.00003 0.00302 0.00654 0.00957 -1.09910

D43 -1.00847 0.00004 0.00405 0.00559 0.00965 -0.99882

D44 1.12215 -0.00001 0.00329 0.00507 0.00835 1.13050

D45 -3.13882 0.00001 0.00362 0.00546 0.00907 -3.12974

D46 3.12603 0.00002 0.00916 0.00120 0.01036 3.13639

D47 -1.06292 0.00007 0.01004 0.00070 0.01074 -1.05217

D48 1.02983 0.00003 0.00933 0.00035 0.00968 1.03951

D49 1.00003 -0.00001 0.00914 0.00181 0.01095 1.01099

D50 3.09427 0.00004 0.01002 0.00131 0.01133 3.10560

D51 -1.09617 0.00000 0.00931 0.00096 0.01027 -1.08590

D52 -1.02913 0.00000 0.00916 0.00160 0.01076 -1.01838

D53 1.06510 0.00005 0.01004 0.00110 0.01114 1.07624

D54 -3.12534 0.00001 0.00932 0.00075 0.01008 -3.11526

Item Value Threshold Converged?

Maximum Force 0.001006 0.000450 NO

RMS Force 0.000175 0.000300 YES

Maximum Displacement 0.099471 0.001800 NO

RMS Displacement 0.028658 0.001200 NO

Predicted change in Energy=-1.575734D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:57:45 2019, MaxMem= 1342177280 cpu: 0.6

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.090787 -0.418217 -0.196356

2 6 0 -2.846792 0.080067 0.474942

3 8 0 -4.904961 0.287922 -0.749920

4 8 0 -4.207113 -1.763876 -0.173658

5 6 0 -2.285143 -0.796246 1.576484

6 16 0 -1.587936 0.316893 -0.944955

7 6 0 -0.120916 0.778510 -0.102717

8 16 0 1.073596 -0.556682 -0.004830

9 16 0 0.031635 2.256834 0.768159

10 6 0 2.680965 0.331109 -0.008276

11 6 0 3.836939 -0.660778 -0.077690

12 6 0 5.195591 0.046159 -0.053677

13 6 0 6.367511 -0.928720 -0.143547

14 1 0 -3.054438 1.087166 0.833304

15 1 0 -5.014067 -1.991289 -0.665452

16 1 0 -1.380817 -0.339443 1.980613

17 1 0 -3.007738 -0.891758 2.393308

18 1 0 -2.036988 -1.794179 1.214987

19 1 0 2.685903 1.001752 -0.870256

20 1 0 2.740061 0.939866 0.893927

21 1 0 3.778114 -1.359323 0.765481

22 1 0 3.756373 -1.263048 -0.989754

23 1 0 5.245774 0.759007 -0.885377

24 1 0 5.280137 0.638679 0.864742

25 1 0 7.326556 -0.402355 -0.129997

26 1 0 6.364774 -1.631787 0.695984

27 1 0 6.325926 -1.517902 -1.065245

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.498817 0.000000

3 O 1.211587 2.404070 0.000000

4 O 1.350868 2.381445 2.242531 0.000000

5 C 2.558558 1.515509 3.667564 2.773675 0.000000

6 S 2.713862 1.912305 3.322880 3.432868 2.843032

7 C 4.147385 2.872614 4.852487 4.813082 3.159660

8 S 5.169787 4.000634 6.083720 5.419567 3.720090

9 S 5.008048 3.620722 5.527310 5.917779 3.916905

10 C 6.815680 5.554513 7.622216 7.201523 5.333350

11 C 7.932324 6.747334 8.818885 8.119902 6.343070

12 C 9.299076 8.059808 10.127406 9.576088 7.702497

13 C 10.470884 9.289971 11.354142 10.607595 8.822952

14 H 2.097712 1.088938 2.563167 3.235903 2.165957

15 H 1.883362 3.207506 2.283384 0.971984 3.728462

16 H 3.476973 2.142922 4.502110 3.828556 1.090777

17 H 2.846682 2.156496 3.856291 2.964524 1.094746

18 H 2.846621 2.171692 4.052317 2.576566 1.090014

19 H 6.956578 5.767996 7.625303 7.459733 5.825001

20 H 7.049368 5.668133 7.846886 7.530815 5.360284

21 H 7.983133 6.785693 8.966919 8.050434 6.143115

22 H 7.932284 6.895729 8.802371 8.020844 6.580532

23 H 9.435675 8.234139 10.162563 9.809615 8.074298

24 H 9.489846 8.155425 10.318255 9.841669 7.732984

25 H 11.417546 10.202729 12.266653 11.613834 9.769953

26 H 10.563511 9.371885 11.523143 10.608416 8.734670

27 H 10.510574 9.437395 11.379510 10.573567 9.036040

6 7 8 9 10

6 S 0.000000

7 C 1.753454 0.000000

8 S 2.954779 1.794207 0.000000

9 S 3.053054 1.722538 3.098236 0.000000

10 C 4.370479 2.838948 1.836252 3.366039 0.000000

11 C 5.580077 4.211507 2.766263 4.869113 1.524773

12 C 6.847183 5.366935 4.166131 5.677054 2.531126

13 C 8.092154 6.709396 5.308785 7.149985 3.898216

14 H 2.430257 3.094665 4.521655 3.300941 5.845915

15 H 4.140555 5.650786 6.289209 6.749881 8.064672

16 H 3.005432 2.679073 3.164383 3.194639 4.572023

17 H 3.823699 4.165775 4.745591 4.668247 6.294788

18 H 3.053460 3.467911 3.563017 4.570510 5.317171

19 H 4.329008 2.918422 2.403583 3.362257 1.092152

20 H 4.743536 3.033896 2.413405 3.014265 1.089976

21 H 5.876204 4.530621 2.924385 5.206986 2.158702

22 H 5.573137 4.470812 2.943862 5.417887 2.158966

23 H 6.848255 5.423495 4.462451 5.671412 2.744202

24 H 7.109780 5.488798 4.458703 5.493135 2.759068

25 H 8.980514 7.540558 6.256116 7.816255 4.704710

26 H 8.350786 6.965029 5.444589 7.432040 4.233129

27 H 8.124663 6.910987 5.443840 7.564925 4.221582

11 12 13 14 15

11 C 0.000000

12 C 1.531755 0.000000

13 C 2.545570 1.527044 0.000000

14 H 7.167726 8.362620 9.684583 0.000000

15 H 8.969728 10.428930 11.442978 3.945035 0.000000

16 H 5.618260 6.894648 8.055799 2.480431 4.788607

17 H 7.280714 8.611739 9.712482 2.520304 3.819730

18 H 6.120346 7.570110 8.557467 3.079453 3.526740

19 H 2.171877 2.806865 4.220079 5.988399 8.263763

20 H 2.170078 2.779621 4.210268 5.796688 8.435036

21 H 1.096523 2.157694 2.777901 7.257662 8.930251

22 H 1.095939 2.159077 2.765120 7.431971 8.806595

23 H 2.157073 1.096538 2.158016 8.482633 10.624350

24 H 2.158607 1.096230 2.157723 8.346692 10.734470

25 H 3.499563 2.178990 1.094079 10.531460 12.454011

26 H 2.816270 2.178183 1.095044 9.804749 11.465633

27 H 2.811580 2.178810 1.094711 9.918774 11.356908

16 17 18 19 20

16 H 0.000000

17 H 1.766987 0.000000

18 H 1.770028 1.773460 0.000000

19 H 5.144363 6.830357 5.871215 0.000000

20 H 4.449624 6.216123 5.513464 1.766098 0.000000

21 H 5.397339 6.994014 5.848638 3.072985 2.525930

22 H 6.005568 7.572065 6.221416 2.507889 3.071477

23 H 7.302890 9.033010 7.998057 2.571399 3.078511

24 H 6.824236 8.565491 7.718924 3.141988 2.558037

25 H 8.959742 10.649142 9.561491 4.904605 4.887321

26 H 7.957047 9.553666 8.419343 4.787768 4.448721

27 H 8.370179 9.973511 8.672607 4.431302 4.768375

21 22 23 24 25

21 H 0.000000

22 H 1.758008 0.000000

23 H 3.060504 2.513547 0.000000

24 H 2.501587 3.062283 1.754587 0.000000

25 H 3.782739 3.771761 2.499803 2.502216 0.000000

26 H 2.601899 3.127529 3.077135 2.521890 1.766005

27 H 3.141345 2.583264 2.526538 3.077233 1.766464

26 27

26 H 0.000000

27 H 1.765334 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 2.88D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.098919 -0.477313 -0.115998

2 6 0 -2.849804 0.123880 0.453855

3 8 0 -4.917071 0.128086 -0.773313

4 8 0 -4.215372 -1.800270 0.131124

5 6 0 -2.280091 -0.557785 1.681670

6 16 0 -1.601599 0.119328 -0.994894

7 6 0 -0.128189 0.712475 -0.252034

8 16 0 1.066725 -0.589579 0.057823

9 16 0 0.031231 2.314856 0.359601

10 6 0 2.674222 0.282900 -0.105129

11 6 0 3.829420 -0.708410 -0.017070

12 6 0 5.188372 -0.009329 -0.121023

13 6 0 6.359366 -0.987296 -0.056082

14 1 0 -3.054526 1.176867 0.641187

15 1 0 -5.026049 -2.105145 -0.310017

16 1 0 -1.372652 -0.041444 1.997489

17 1 0 -2.996551 -0.515009 2.508304

18 1 0 -2.034883 -1.602315 1.489422

19 1 0 2.672834 0.800784 -1.066685

20 1 0 2.740231 1.033184 0.682758

21 1 0 3.776775 -1.256856 0.930980

22 1 0 3.741869 -1.453906 -0.815601

23 1 0 5.232464 0.555142 -1.060078

24 1 0 5.279949 0.727604 0.685367

25 1 0 7.318603 -0.467423 -0.137364

26 1 0 6.362778 -1.540889 0.888718

27 1 0 6.310725 -1.721546 -0.866577

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2977721 0.1940566 0.1812350

Leave Link 202 at Sat Aug 17 17:57:45 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.7601947577 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0550382238 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.7051565339 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

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Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2325

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.10D-08

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 95

GePol: Fraction of low-weight points (<1% of avg) = 4.09%

GePol: Cavity surface area = 308.972 Ang\*\*2

GePol: Cavity volume = 320.241 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057942529 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.6993622810 Hartrees.

Leave Link 301 at Sat Aug 17 17:57:45 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:57:46 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:57:46 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999978 0.006692 -0.000044 -0.000036 Ang= 0.77 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.63027916681

Leave Link 401 at Sat Aug 17 17:57:46 2019, MaxMem= 1342177280 cpu: 7.6

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16216875.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.11D-15 for 2286.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.41D-15 for 750 507.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.11D-15 for 2286.

Iteration 1 A^-1\*A deviation from orthogonality is 3.59D-11 for 643 556.

E= -1658.67507396241

DIIS: error= 1.25D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67507396241 IErMin= 1 ErrMin= 1.25D-03

ErrMax= 1.25D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.87D-03 BMatP= 4.87D-03

IDIUse=3 WtCom= 9.88D-01 WtEn= 1.25D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.428 Goal= None Shift= 0.000

Gap= 0.484 Goal= None Shift= 0.000

GapD= 0.428 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=1.50D-04 MaxDP=3.53D-03 OVMax= 9.76D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.50D-04 CP: 1.00D+00

E= -1658.67697407136 Delta-E= -0.001900108948 Rises=F Damp=F

DIIS: error= 2.04D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67697407136 IErMin= 2 ErrMin= 2.04D-04

ErrMax= 2.04D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.67D-05 BMatP= 4.87D-03

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.04D-03

Coeff-Com: -0.544D-01 0.105D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.543D-01 0.105D+01

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.74D-05 MaxDP=9.35D-04 DE=-1.90D-03 OVMax= 1.68D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.65D-05 CP: 1.00D+00 1.04D+00

E= -1658.67698565393 Delta-E= -0.000011582570 Rises=F Damp=F

DIIS: error= 3.45D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67698565393 IErMin= 2 ErrMin= 2.04D-04

ErrMax= 3.45D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.86D-05 BMatP= 8.67D-05

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.45D-03

Coeff-Com: -0.365D-01 0.543D+00 0.494D+00

Coeff-En: 0.000D+00 0.233D+00 0.767D+00

Coeff: -0.363D-01 0.542D+00 0.495D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.38D-05 MaxDP=6.61D-04 DE=-1.16D-05 OVMax= 1.29D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 8.26D-06 CP: 1.00D+00 1.07D+00 6.07D-01

E= -1658.67699851149 Delta-E= -0.000012857557 Rises=F Damp=F

DIIS: error= 1.70D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67699851149 IErMin= 4 ErrMin= 1.70D-04

ErrMax= 1.70D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.28D-05 BMatP= 7.86D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.70D-03

Coeff-Com: -0.132D-01 0.180D+00 0.302D+00 0.532D+00

Coeff-En: 0.000D+00 0.000D+00 0.107D+00 0.893D+00

Coeff: -0.131D-01 0.180D+00 0.301D+00 0.532D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.76D-06 MaxDP=1.94D-04 DE=-1.29D-05 OVMax= 5.33D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.74D-06 CP: 1.00D+00 1.07D+00 6.47D-01 6.92D-01

E= -1658.67700053645 Delta-E= -0.000002024961 Rises=F Damp=F

DIIS: error= 4.19D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67700053645 IErMin= 5 ErrMin= 4.19D-05

ErrMax= 4.19D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.40D-06 BMatP= 1.28D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.449D-02 0.571D-01 0.138D+00 0.324D+00 0.485D+00

Coeff: -0.449D-02 0.571D-01 0.138D+00 0.324D+00 0.485D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.55D-06 MaxDP=8.10D-05 DE=-2.02D-06 OVMax= 1.40D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.20D-06 CP: 1.00D+00 1.07D+00 6.62D-01 7.68D-01 8.33D-01

E= -1658.67700078728 Delta-E= -0.000000250830 Rises=F Damp=F

DIIS: error= 8.39D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67700078728 IErMin= 6 ErrMin= 8.39D-06

ErrMax= 8.39D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.03D-07 BMatP= 1.40D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.116D-03-0.599D-02 0.156D-01 0.700D-01 0.241D+00 0.680D+00

Coeff: 0.116D-03-0.599D-02 0.156D-01 0.700D-01 0.241D+00 0.680D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=8.13D-07 MaxDP=5.95D-05 DE=-2.51D-07 OVMax= 9.05D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.52D-07 CP: 1.00D+00 1.07D+00 6.82D-01 7.94D-01 8.80D-01

CP: 9.41D-01

E= -1658.67700080965 Delta-E= -0.000000022369 Rises=F Damp=F

DIIS: error= 2.68D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67700080965 IErMin= 7 ErrMin= 2.68D-06

ErrMax= 2.68D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.18D-08 BMatP= 1.03D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.543D-03-0.933D-02-0.735D-02-0.736D-03 0.609D-01 0.317D+00

Coeff-Com: 0.639D+00

Coeff: 0.543D-03-0.933D-02-0.735D-02-0.736D-03 0.609D-01 0.317D+00

Coeff: 0.639D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.86D-07 MaxDP=1.01D-05 DE=-2.24D-08 OVMax= 3.42D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.10D-07 CP: 1.00D+00 1.07D+00 6.82D-01 8.07D-01 9.12D-01

CP: 1.02D+00 1.01D+00

E= -1658.67700081313 Delta-E= -0.000000003480 Rises=F Damp=F

DIIS: error= 9.18D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67700081313 IErMin= 8 ErrMin= 9.18D-07

ErrMax= 9.18D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.55D-09 BMatP= 1.18D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.180D-03-0.253D-02-0.498D-02-0.101D-01-0.106D-01 0.231D-01

Coeff-Com: 0.259D+00 0.746D+00

Coeff: 0.180D-03-0.253D-02-0.498D-02-0.101D-01-0.106D-01 0.231D-01

Coeff: 0.259D+00 0.746D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.98D-07 MaxDP=1.05D-05 DE=-3.48D-09 OVMax= 3.32D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 9.48D-08 CP: 1.00D+00 1.07D+00 6.84D-01 8.12D-01 9.30D-01

CP: 1.09D+00 1.20D+00 1.05D+00

E= -1658.67700081386 Delta-E= -0.000000000735 Rises=F Damp=F

DIIS: error= 6.09D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67700081386 IErMin= 9 ErrMin= 6.09D-07

ErrMax= 6.09D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.25D-10 BMatP= 1.55D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.304D-04 0.896D-03-0.892D-03-0.497D-02-0.191D-01-0.599D-01

Coeff-Com: -0.287D-01 0.358D+00 0.755D+00

Coeff: -0.304D-04 0.896D-03-0.892D-03-0.497D-02-0.191D-01-0.599D-01

Coeff: -0.287D-01 0.358D+00 0.755D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=8.84D-08 MaxDP=4.45D-06 DE=-7.35D-10 OVMax= 9.97D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 4.15D-08 CP: 1.00D+00 1.07D+00 6.85D-01 8.15D-01 9.35D-01

CP: 1.11D+00 1.29D+00 1.24D+00 8.35D-01

E= -1658.67700081407 Delta-E= -0.000000000204 Rises=F Damp=F

DIIS: error= 2.52D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67700081407 IErMin=10 ErrMin= 2.52D-07

ErrMax= 2.52D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.19D-10 BMatP= 4.25D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.488D-04 0.967D-03 0.360D-03-0.101D-02-0.879D-02-0.375D-01

Coeff-Com: -0.630D-01 0.775D-01 0.442D+00 0.589D+00

Coeff: -0.488D-04 0.967D-03 0.360D-03-0.101D-02-0.879D-02-0.375D-01

Coeff: -0.630D-01 0.775D-01 0.442D+00 0.589D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.55D-08 MaxDP=2.24D-06 DE=-2.04D-10 OVMax= 6.93D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.86D-08 CP: 1.00D+00 1.07D+00 6.85D-01 8.16D-01 9.37D-01

CP: 1.13D+00 1.33D+00 1.32D+00 1.03D+00 6.82D-01

E= -1658.67700081409 Delta-E= -0.000000000026 Rises=F Damp=F

DIIS: error= 1.25D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67700081409 IErMin=11 ErrMin= 1.25D-07

ErrMax= 1.25D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.38D-11 BMatP= 1.19D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.222D-04 0.383D-03 0.339D-03 0.268D-03-0.162D-02-0.107D-01

Coeff-Com: -0.323D-01-0.201D-01 0.117D+00 0.344D+00 0.603D+00

Coeff: -0.222D-04 0.383D-03 0.339D-03 0.268D-03-0.162D-02-0.107D-01

Coeff: -0.323D-01-0.201D-01 0.117D+00 0.344D+00 0.603D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.20D-08 MaxDP=8.27D-07 DE=-2.59D-11 OVMax= 2.26D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 7.75D-09 CP: 1.00D+00 1.07D+00 6.85D-01 8.16D-01 9.37D-01

CP: 1.13D+00 1.33D+00 1.34D+00 1.06D+00 8.10D-01

CP: 8.19D-01

E= -1658.67700081409 Delta-E= 0.000000000005 Rises=F Damp=F

DIIS: error= 4.52D-08 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=11 EnMin= -1658.67700081409 IErMin=12 ErrMin= 4.52D-08

ErrMax= 4.52D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.76D-12 BMatP= 2.38D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.138D-05-0.138D-04 0.109D-03 0.404D-03 0.122D-02 0.315D-02

Coeff-Com: -0.328D-02-0.315D-01-0.445D-01 0.500D-01 0.348D+00 0.677D+00

Coeff: -0.138D-05-0.138D-04 0.109D-03 0.404D-03 0.122D-02 0.315D-02

Coeff: -0.328D-02-0.315D-01-0.445D-01 0.500D-01 0.348D+00 0.677D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.81D-09 MaxDP=3.43D-07 DE= 5.46D-12 OVMax= 7.27D-07

Error on total polarization charges = 0.04159

SCF Done: E(UB3LYP) = -1658.67700081 A.U. after 12 cycles

NFock= 12 Conv=0.68D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655240884215D+03 PE=-6.148166245091D+03 EE= 1.731548997781D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.64

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:58:13 2019, MaxMem= 1342177280 cpu: 305.7

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 337

Leave Link 701 at Sat Aug 17 17:58:14 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:58:14 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:58:17 2019, MaxMem= 1342177280 cpu: 38.7

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.42990269D+00-2.96070697D+00 6.48553827D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000059021 -0.000025354 -0.000517385

2 6 0.000127020 0.000547005 -0.000080403

3 8 -0.000355119 -0.000030887 0.000031185

4 8 -0.000352572 -0.000080766 -0.000099274

5 6 0.000234223 0.000261988 0.000271611

6 16 0.000239769 -0.000091499 -0.000066610

7 6 0.000297377 0.000078073 0.000009765

8 16 -0.000427034 0.000191091 0.000146274

9 16 -0.000102942 -0.000406580 -0.000088001

10 6 0.000076050 0.000004305 -0.000123323

11 6 0.000080171 0.000297002 0.000161402

12 6 -0.000149549 -0.000117801 -0.000287151

13 6 0.000056586 0.000002280 0.000191278

14 1 0.000093595 -0.000155514 0.000593948

15 1 -0.000041907 -0.000161207 -0.000001842

16 1 -0.000012603 -0.000143539 0.000135477

17 1 -0.000004830 -0.000139248 -0.000091557

18 1 -0.000080581 -0.000066845 -0.000051383

19 1 0.000172744 0.000150761 -0.000081675

20 1 -0.000000395 -0.000062356 0.000178288

21 1 -0.000023311 -0.000055667 -0.000065165

22 1 0.000023977 -0.000007201 -0.000039260

23 1 0.000021696 -0.000006909 0.000074276

24 1 -0.000066592 0.000042932 0.000040442

25 1 0.000095160 -0.000080096 -0.000071235

26 1 0.000013878 0.000027661 -0.000008967

27 1 0.000026168 0.000028372 -0.000160715

-------------------------------------------------------------------

Cartesian Forces: Max 0.000593948 RMS 0.000179521

Leave Link 716 at Sat Aug 17 17:58:17 2019, MaxMem= 1342177280 cpu: 0.3

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000938550 RMS 0.000163297

Search for a local minimum.

Step number 61 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .16330D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43 45 44 47 46

49 48 51 50 53

54 55 56 52 57

59 60 61

DE= 4.63D-05 DEPred=-1.58D-05 R=-2.94D+00

Trust test=-2.94D+00 RLast= 1.10D-01 DXMaxT set to 5.03D-02

ITU= -1 1 0 -1 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 1

ITU= 1 1 -1 -1 0 -1 -1 -1 0 -1 0 0 -1 -1 0 0 -1 0 0 -1

ITU= 1 -1 1 -1 1 1 -1 1 -1 1 1 -1 0 0 -1 0 0 -1 -1 0

ITU= 0

Eigenvalues --- 0.00043 0.00099 0.00161 0.00225 0.00273

Eigenvalues --- 0.00312 0.00390 0.00680 0.01624 0.01821

Eigenvalues --- 0.02670 0.03481 0.03623 0.03771 0.04274

Eigenvalues --- 0.04569 0.04799 0.04947 0.04999 0.05252

Eigenvalues --- 0.05400 0.05458 0.05608 0.05815 0.07461

Eigenvalues --- 0.08120 0.08310 0.10814 0.11070 0.11458

Eigenvalues --- 0.12107 0.12378 0.13765 0.14998 0.15335

Eigenvalues --- 0.15842 0.16143 0.16187 0.16672 0.17255

Eigenvalues --- 0.18454 0.18843 0.20526 0.21581 0.22104

Eigenvalues --- 0.22702 0.23204 0.24892 0.25464 0.26978

Eigenvalues --- 0.27571 0.28395 0.28957 0.29517 0.30011

Eigenvalues --- 0.30887 0.31352 0.33424 0.33689 0.33839

Eigenvalues --- 0.33875 0.33956 0.34008 0.34035 0.34064

Eigenvalues --- 0.34141 0.34224 0.34249 0.34669 0.35121

Eigenvalues --- 0.35438 0.35871 0.46668 0.52522 0.88798

En-DIIS/RFO-DIIS IScMMF= 0 using points: 61 60 59

RFO step: Lambda=-8.78479464D-06.

NNeg= 0 NP= 3 Switch= 2.50D-03 Rises=F DC= 2.86D-05 SmlDif= 1.00D-05

RMS Error= 0.5637191859D-03 NUsed= 3 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.06216 0.05158 0.88625

Iteration 1 RMS(Cart)= 0.01880766 RMS(Int)= 0.00010271

Iteration 2 RMS(Cart)= 0.00017634 RMS(Int)= 0.00000059

Iteration 3 RMS(Cart)= 0.00000002 RMS(Int)= 0.00000059

ITry= 1 IFail=0 DXMaxC= 6.00D-02 DCOld= 1.00D+10 DXMaxT= 5.03D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83235 0.00094 0.00319 0.00042 0.00361 2.83596

R2 2.28957 0.00020 -0.00043 -0.00002 -0.00045 2.28912

R3 2.55277 0.00031 0.00020 0.00049 0.00069 2.55346

R4 2.86390 0.00023 0.00120 -0.00015 0.00105 2.86494

R5 3.61373 0.00038 -0.00269 -0.00110 -0.00379 3.60995

R6 2.05780 0.00003 0.00026 -0.00022 0.00004 2.05784

R7 1.83678 0.00006 0.00011 -0.00003 0.00007 1.83686

R8 2.06127 0.00000 0.00004 -0.00021 -0.00017 2.06110

R9 2.06877 -0.00005 -0.00010 -0.00002 -0.00012 2.06865

R10 2.05983 0.00002 0.00018 -0.00019 0.00000 2.05982

R11 3.31355 0.00002 0.00137 0.00109 0.00246 3.31601

R12 3.39056 -0.00031 -0.00255 -0.00020 -0.00275 3.38781

R13 3.25513 -0.00042 -0.00118 0.00009 -0.00109 3.25404

R14 3.47001 0.00036 0.00207 -0.00025 0.00182 3.47183

R15 2.88140 0.00002 0.00001 -0.00006 -0.00005 2.88135

R16 2.06387 0.00017 0.00037 0.00015 0.00053 2.06439

R17 2.05976 0.00010 0.00027 0.00003 0.00029 2.06005

R18 2.89460 -0.00007 -0.00046 -0.00006 -0.00052 2.89408

R19 2.07213 0.00000 0.00006 0.00005 0.00011 2.07224

R20 2.07102 0.00003 0.00012 0.00007 0.00019 2.07122

R21 2.88570 0.00018 0.00045 -0.00014 0.00031 2.88600

R22 2.07216 -0.00006 -0.00024 0.00011 -0.00013 2.07203

R23 2.07157 0.00005 0.00022 -0.00004 0.00018 2.07176

R24 2.06751 0.00004 0.00013 0.00000 0.00013 2.06764

R25 2.06933 0.00000 -0.00009 0.00010 0.00001 2.06934

R26 2.06870 0.00010 0.00035 -0.00008 0.00027 2.06897

A1 2.17562 0.00019 0.00066 -0.00028 0.00037 2.17599

A2 1.97699 0.00018 0.00053 -0.00015 0.00037 1.97736

A3 2.12985 -0.00035 -0.00104 0.00045 -0.00059 2.12926

A4 2.02740 0.00002 -0.00004 -0.00053 -0.00057 2.02683

A5 1.82863 -0.00007 0.00099 0.00077 0.00176 1.83039

A6 1.87192 0.00019 0.00140 -0.00035 0.00105 1.87297

A7 1.94694 0.00004 -0.00046 0.00079 0.00032 1.94726

A8 1.94576 -0.00034 -0.00420 -0.00055 -0.00475 1.94101

A9 1.82900 0.00022 0.00298 -0.00005 0.00293 1.83193

A10 1.87136 0.00033 0.00095 -0.00007 0.00089 1.87224

A11 1.91176 0.00027 0.00109 0.00009 0.00118 1.91294

A12 1.92640 -0.00004 0.00005 -0.00044 -0.00039 1.92601

A13 1.95271 -0.00010 -0.00042 0.00007 -0.00035 1.95237

A14 1.88318 -0.00007 0.00026 0.00001 0.00027 1.88345

A15 1.89393 -0.00004 0.00022 0.00040 0.00062 1.89455

A16 1.89425 -0.00003 -0.00119 -0.00013 -0.00132 1.89293

A17 1.79950 0.00046 -0.00087 -0.00029 -0.00115 1.79834

A18 1.96850 0.00026 0.00149 0.00018 0.00167 1.97017

A19 2.14465 -0.00019 -0.00161 -0.00022 -0.00183 2.14283

A20 2.15570 -0.00009 -0.00054 0.00005 -0.00049 2.15521

A21 1.79557 0.00029 0.00021 0.00017 0.00038 1.79595

A22 1.92752 -0.00006 -0.00081 -0.00099 -0.00180 1.92572

A23 1.87792 0.00014 0.00119 0.00107 0.00226 1.88018

A24 1.89224 0.00001 -0.00033 -0.00082 -0.00115 1.89109

A25 1.93917 -0.00006 0.00025 0.00013 0.00038 1.93955

A26 1.93895 -0.00006 -0.00085 0.00025 -0.00061 1.93834

A27 1.88608 0.00005 0.00062 0.00039 0.00101 1.88709

A28 1.95143 0.00019 0.00136 0.00025 0.00161 1.95304

A29 1.91637 -0.00011 -0.00037 -0.00062 -0.00100 1.91537

A30 1.91733 0.00002 -0.00002 0.00024 0.00022 1.91755

A31 1.90662 0.00001 0.00027 0.00011 0.00038 1.90699

A32 1.90909 -0.00012 -0.00066 0.00024 -0.00042 1.90867

A33 1.86074 0.00001 -0.00067 -0.00023 -0.00090 1.85984

A34 1.96617 0.00005 -0.00008 -0.00017 -0.00024 1.96593

A35 1.90576 0.00000 0.00037 0.00040 0.00077 1.90652

A36 1.90816 -0.00006 -0.00033 -0.00011 -0.00044 1.90772

A37 1.91268 0.00000 0.00021 0.00023 0.00044 1.91312

A38 1.91260 0.00001 0.00013 -0.00028 -0.00015 1.91245

A39 1.85516 0.00000 -0.00032 -0.00006 -0.00038 1.85477

A40 1.94427 0.00018 0.00115 0.00001 0.00115 1.94543

A41 1.94212 -0.00004 -0.00010 0.00028 0.00018 1.94230

A42 1.94335 -0.00004 -0.00042 -0.00003 -0.00045 1.94290

A43 1.87715 -0.00006 -0.00018 -0.00017 -0.00035 1.87680

A44 1.87828 -0.00010 -0.00101 -0.00009 -0.00111 1.87717

A45 1.87533 0.00005 0.00053 -0.00001 0.00052 1.87585

D1 2.69976 -0.00019 0.01225 -0.01070 0.00155 2.70131

D2 -1.42692 -0.00019 0.01239 -0.00944 0.00295 -1.42397

D3 0.51045 0.00010 0.01673 -0.00930 0.00743 0.51787

D4 -0.48220 0.00000 0.01663 -0.01038 0.00624 -0.47595

D5 1.67431 0.00000 0.01676 -0.00912 0.00764 1.68195

D6 -2.67151 0.00029 0.02110 -0.00898 0.01212 -2.65939

D7 -3.09475 -0.00014 -0.00459 -0.00129 -0.00588 -3.10063

D8 0.00767 0.00007 -0.00031 -0.00099 -0.00130 0.00637

D9 3.13159 0.00001 0.00778 0.00569 0.01347 -3.13813

D10 -1.08056 0.00007 0.00881 0.00549 0.01430 -1.06626

D11 1.03072 -0.00007 0.00704 0.00508 0.01212 1.04283

D12 1.03783 0.00007 0.00685 0.00443 0.01128 1.04910

D13 3.10887 0.00013 0.00788 0.00422 0.01210 3.12097

D14 -1.06305 -0.00001 0.00611 0.00381 0.00993 -1.05312

D15 -1.00028 -0.00001 0.00611 0.00434 0.01045 -0.98983

D16 1.07076 0.00005 0.00714 0.00413 0.01128 1.08204

D17 -3.10115 -0.00009 0.00537 0.00372 0.00910 -3.09205

D18 -3.06845 -0.00004 -0.01921 0.00077 -0.01844 -3.08689

D19 -0.86114 -0.00005 -0.01887 0.00113 -0.01773 -0.87887

D20 1.24667 -0.00031 -0.02234 0.00087 -0.02147 1.22520

D21 1.81578 -0.00003 0.00586 -0.00164 0.00422 1.82000

D22 -1.15031 0.00005 0.00982 -0.00173 0.00808 -1.14223

D23 2.60494 -0.00008 -0.01077 -0.00400 -0.01477 2.59017

D24 -0.71344 -0.00017 -0.01489 -0.00393 -0.01882 -0.73226

D25 -3.03727 -0.00008 0.00536 -0.00447 0.00089 -3.03638

D26 -0.91804 -0.00010 0.00593 -0.00422 0.00170 -0.91634

D27 1.11782 0.00003 0.00712 -0.00363 0.00349 1.12131

D28 -3.12143 0.00000 -0.00195 0.00103 -0.00093 -3.12235

D29 -1.00224 0.00006 -0.00096 0.00089 -0.00007 -1.00231

D30 1.03877 0.00002 -0.00201 0.00039 -0.00162 1.03715

D31 1.07924 -0.00010 -0.00307 0.00025 -0.00282 1.07642

D32 -3.08476 -0.00003 -0.00208 0.00012 -0.00197 -3.08672

D33 -1.04375 -0.00008 -0.00313 -0.00039 -0.00352 -1.04727

D34 -1.02110 -0.00008 -0.00346 -0.00050 -0.00396 -1.02506

D35 1.09808 -0.00001 -0.00247 -0.00063 -0.00310 1.09498

D36 3.13909 -0.00006 -0.00352 -0.00114 -0.00465 3.13444

D37 -3.12655 -0.00007 -0.00561 0.00064 -0.00497 -3.13153

D38 -0.99723 -0.00003 -0.00513 0.00110 -0.00403 -1.00126

D39 1.02571 -0.00007 -0.00549 0.00118 -0.00431 1.02140

D40 1.03182 -0.00006 -0.00622 0.00119 -0.00503 1.02679

D41 -3.12204 -0.00003 -0.00574 0.00165 -0.00409 -3.12612

D42 -1.09910 -0.00007 -0.00610 0.00174 -0.00436 -1.10346

D43 -0.99882 -0.00001 -0.00519 0.00127 -0.00392 -1.00274

D44 1.13050 0.00002 -0.00471 0.00173 -0.00298 1.12753

D45 -3.12974 -0.00001 -0.00507 0.00182 -0.00325 -3.13300

D46 3.13639 0.00000 -0.00101 0.00945 0.00844 -3.13835

D47 -1.05217 0.00002 -0.00053 0.00943 0.00890 -1.04328

D48 1.03951 0.00003 -0.00021 0.00958 0.00937 1.04889

D49 1.01099 -0.00004 -0.00158 0.00889 0.00732 1.01830

D50 3.10560 -0.00002 -0.00110 0.00887 0.00777 3.11337

D51 -1.08590 -0.00001 -0.00078 0.00903 0.00825 -1.07765

D52 -1.01838 -0.00003 -0.00139 0.00900 0.00761 -1.01077

D53 1.07624 -0.00002 -0.00091 0.00897 0.00806 1.08431

D54 -3.11526 0.00000 -0.00059 0.00913 0.00854 -3.10672

Item Value Threshold Converged?

Maximum Force 0.000939 0.000450 NO

RMS Force 0.000163 0.000300 YES

Maximum Displacement 0.060047 0.001800 NO

RMS Displacement 0.018784 0.001200 NO

Predicted change in Energy=-1.737360D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:58:17 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.095247 -0.406986 -0.201258

2 6 0 -2.843915 0.073717 0.473484

3 8 0 -4.898415 0.310535 -0.755746

4 8 0 -4.234053 -1.750814 -0.174952

5 6 0 -2.296024 -0.813191 1.574237

6 16 0 -1.579924 0.299591 -0.940928

7 6 0 -0.117250 0.770033 -0.093321

8 16 0 1.081830 -0.558056 0.017768

9 16 0 0.021722 2.250554 0.774955

10 6 0 2.686993 0.335322 -0.008403

11 6 0 3.844050 -0.655732 -0.070726

12 6 0 5.202581 0.051240 -0.066822

13 6 0 6.373922 -0.925752 -0.143033

14 1 0 -3.039334 1.080586 0.839351

15 1 0 -5.045842 -1.966722 -0.664043

16 1 0 -1.393649 -0.364096 1.990928

17 1 0 -3.027214 -0.912052 2.382891

18 1 0 -2.049921 -1.809816 1.207771

19 1 0 2.686299 0.995082 -0.879103

20 1 0 2.749623 0.954828 0.886400

21 1 0 3.790705 -1.341607 0.783216

22 1 0 3.758038 -1.272507 -0.972665

23 1 0 5.249353 0.748565 -0.911687

24 1 0 5.291240 0.660976 0.839982

25 1 0 7.334037 -0.401078 -0.135709

26 1 0 6.369890 -1.618150 0.705316

27 1 0 6.332666 -1.526107 -1.057680

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.500728 0.000000

3 O 1.211351 2.405838 0.000000

4 O 1.351234 2.383666 2.242288 0.000000

5 C 2.560193 1.516063 3.669334 2.773942 0.000000

6 S 2.715367 1.910302 3.323672 3.440245 2.842031

7 C 4.149878 2.870684 4.848658 4.827981 3.167713

8 S 5.183910 4.002285 6.092299 5.451461 3.727947

9 S 4.996494 3.611285 5.505858 5.918183 3.923944

10 C 6.825467 5.558021 7.622175 7.230531 5.352970

11 C 7.944265 6.749602 8.822336 8.152657 6.358554

12 C 9.310084 8.064648 10.127783 9.607766 7.724597

13 C 10.482177 9.292339 11.356470 10.640061 8.839099

14 H 2.100164 1.088959 2.567780 3.236200 2.163090

15 H 1.884298 3.210271 2.283866 0.972023 3.728542

16 H 3.479390 2.144199 4.503635 3.831699 1.090687

17 H 2.841410 2.156658 3.853200 2.950007 1.094684

18 H 2.852483 2.171935 4.057734 2.585699 1.090012

19 H 6.958063 5.767293 7.616541 7.478438 5.840571

20 H 7.063271 5.677546 7.848837 7.564304 5.390508

21 H 8.001934 6.790969 8.977682 8.092112 6.160618

22 H 7.938406 6.891259 8.802684 8.046033 6.584022

23 H 9.442541 8.238635 10.158415 9.834870 8.096396

24 H 9.504255 8.164554 10.319797 9.878159 7.763947

25 H 11.429474 10.207216 12.268811 11.646632 9.789374

26 H 10.573925 9.370719 11.525156 10.641245 8.746488

27 H 10.522703 9.439997 11.384270 10.605907 9.049283

6 7 8 9 10

6 S 0.000000

7 C 1.754755 0.000000

8 S 2.956279 1.792751 0.000000

9 S 3.052177 1.721964 3.096038 0.000000

10 C 4.367775 2.839008 1.837215 3.374231 0.000000

11 C 5.575785 4.210132 2.765362 4.875640 1.524747

12 C 6.843107 5.368238 4.166412 5.690947 2.532252

13 C 8.087136 6.709209 5.307288 7.161150 3.898959

14 H 2.430890 3.083001 4.510448 3.277657 5.836516

15 H 4.150353 5.666266 6.324363 6.748062 8.094814

16 H 3.011803 2.694353 3.171589 3.212206 4.597625

17 H 3.822368 4.174797 4.754299 4.677986 6.318733

18 H 3.047524 3.476159 3.576433 4.578825 5.340323

19 H 4.322983 2.920272 2.406436 3.378178 1.092430

20 H 4.744833 3.035287 2.413478 3.022047 1.090130

21 H 5.874509 4.527633 2.921963 5.206623 2.157992

22 H 5.564740 4.468006 2.941681 5.424592 2.159179

23 H 6.844082 5.428685 4.465355 5.694635 2.748160

24 H 7.107399 5.489509 4.458835 5.504435 2.758244

25 H 8.977639 7.542876 6.256060 7.831373 4.706752

26 H 8.341906 6.958752 5.436920 7.434444 4.229560

27 H 8.121322 6.914020 5.446558 7.579560 4.225735

11 12 13 14 15

11 C 0.000000

12 C 1.531480 0.000000

13 C 2.545269 1.527207 0.000000

14 H 7.157095 8.355230 9.674702 0.000000

15 H 9.005604 10.462267 11.478941 3.946182 0.000000

16 H 5.636396 6.922218 8.074926 2.474169 4.791221

17 H 7.300698 8.640518 9.734570 2.520569 3.804076

18 H 6.140468 7.595189 8.577143 3.077190 3.536079

19 H 2.172337 2.807547 4.222555 5.978567 8.282786

20 H 2.169738 2.782465 4.210922 5.790514 8.468094

21 H 1.096580 2.157772 2.775587 7.247041 8.976074

22 H 1.096040 2.158602 2.766113 7.417864 8.836599

23 H 2.157346 1.096470 2.158430 8.478131 10.650125

24 H 2.158117 1.096327 2.157829 8.341135 10.771358

25 H 3.499869 2.180009 1.094147 10.523920 12.489667

26 H 2.812181 2.178456 1.095047 9.789517 11.502851

27 H 2.815110 2.178741 1.094854 9.911002 11.393838

16 17 18 19 20

16 H 0.000000

17 H 1.767038 0.000000

18 H 1.770349 1.772566 0.000000

19 H 5.170147 6.849963 5.886788 0.000000

20 H 4.486229 6.252725 5.548167 1.767097 0.000000

21 H 5.412174 7.016231 5.874724 3.072968 2.523512

22 H 6.012319 7.578214 6.226988 2.509849 3.071489

23 H 7.334349 9.061648 8.019777 2.575089 3.086148

24 H 6.860262 8.605327 7.754529 3.138885 2.558968

25 H 8.983121 10.675203 9.583744 4.909518 4.888766

26 H 7.968563 9.571750 8.436967 4.786253 4.445148

27 H 8.386908 9.991093 8.687952 4.436697 4.772073

21 22 23 24 25

21 H 0.000000

22 H 1.757543 0.000000

23 H 3.060909 2.512463 0.000000

24 H 2.503031 3.061822 1.754358 0.000000

25 H 3.779447 3.774607 2.503942 2.500590 0.000000

26 H 2.595138 3.123598 3.077603 2.525081 1.765833

27 H 3.143963 2.588484 2.523690 3.077177 1.765918

26 27

26 H 0.000000

27 H 1.765790 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 9.15D-04

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.103736 -0.466659 -0.126538

2 6 0 -2.847302 0.117459 0.449972

3 8 0 -4.910913 0.150173 -0.786351

4 8 0 -4.242569 -1.787346 0.123150

5 6 0 -2.291331 -0.575524 1.678434

6 16 0 -1.593904 0.104013 -0.991578

7 6 0 -0.124842 0.706364 -0.244453

8 16 0 1.074811 -0.586636 0.076388

9 16 0 0.020883 2.310115 0.365389

10 6 0 2.679885 0.287787 -0.109302

11 6 0 3.836273 -0.701520 -0.015022

12 6 0 5.194917 -0.005594 -0.138343

13 6 0 6.365488 -0.983355 -0.060194

14 1 0 -3.039803 1.171314 0.645331

15 1 0 -5.058036 -2.080183 -0.317404

16 1 0 -1.385783 -0.064853 2.008277

17 1 0 -3.016458 -0.537968 2.497649

18 1 0 -2.048149 -1.619448 1.480415

19 1 0 2.672779 0.794119 -1.077279

20 1 0 2.749322 1.046935 0.669964

21 1 0 3.789212 -1.236308 0.941155

22 1 0 3.743402 -1.459125 -0.801605

23 1 0 5.235476 0.541999 -1.087418

24 1 0 5.290470 0.745872 0.654186

25 1 0 7.325719 -0.466076 -0.146996

26 1 0 6.367694 -1.525572 0.891186

27 1 0 6.317278 -1.726935 -0.862360

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3032686 0.1935155 0.1808907

Leave Link 202 at Sat Aug 17 17:58:17 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.3279952789 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0549994832 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.2729957957 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

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Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2324

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.34D-10

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 98

GePol: Fraction of low-weight points (<1% of avg) = 4.22%

GePol: Cavity surface area = 309.270 Ang\*\*2

GePol: Cavity volume = 320.466 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057858661 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.2672099296 Hartrees.

Leave Link 301 at Sat Aug 17 17:58:17 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:58:18 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:58:18 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000772 0.000287 0.000039 Ang= -0.09 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.63013352774

Leave Link 401 at Sat Aug 17 17:58:18 2019, MaxMem= 1342177280 cpu: 7.7

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16202928.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.55D-15 for 706.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.69D-15 for 883 415.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.11D-15 for 2294.

Iteration 1 A^-1\*A deviation from orthogonality is 2.70D-10 for 696 681.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.55D-15 for 84.

Iteration 2 A\*A^-1 deviation from orthogonality is 4.05D-15 for 681 330.

Iteration 2 A^-1\*A deviation from unit magnitude is 9.99D-16 for 1152.

Iteration 2 A^-1\*A deviation from orthogonality is 4.36D-16 for 962 9.

E= -1658.67628901401

DIIS: error= 7.30D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67628901401 IErMin= 1 ErrMin= 7.30D-04

ErrMax= 7.30D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.64D-03 BMatP= 1.64D-03

IDIUse=3 WtCom= 9.93D-01 WtEn= 7.30D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.428 Goal= None Shift= 0.000

Gap= 0.484 Goal= None Shift= 0.000

RMSDP=9.58D-05 MaxDP=3.45D-03 OVMax= 5.89D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 9.58D-05 CP: 1.00D+00

E= -1658.67700596413 Delta-E= -0.000716950118 Rises=F Damp=F

DIIS: error= 9.25D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67700596413 IErMin= 2 ErrMin= 9.25D-05

ErrMax= 9.25D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.65D-05 BMatP= 1.64D-03

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.596D-01 0.106D+01

Coeff: -0.596D-01 0.106D+01

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.58D-05 MaxDP=4.50D-04 DE=-7.17D-04 OVMax= 9.59D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.50D-05 CP: 1.00D+00 1.05D+00

E= -1658.67701259971 Delta-E= -0.000006635582 Rises=F Damp=F

DIIS: error= 9.80D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67701259971 IErMin= 2 ErrMin= 9.25D-05

ErrMax= 9.80D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.36D-05 BMatP= 2.65D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.324D-01 0.463D+00 0.569D+00

Coeff: -0.324D-01 0.463D+00 0.569D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=8.91D-06 MaxDP=3.33D-04 DE=-6.64D-06 OVMax= 1.01D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 6.93D-06 CP: 1.00D+00 1.09D+00 6.91D-01

E= -1658.67701483473 Delta-E= -0.000002235021 Rises=F Damp=F

DIIS: error= 6.11D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67701483473 IErMin= 4 ErrMin= 6.11D-05

ErrMax= 6.11D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.15D-06 BMatP= 1.36D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.121D-01 0.157D+00 0.366D+00 0.489D+00

Coeff: -0.121D-01 0.157D+00 0.366D+00 0.489D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.53D-06 MaxDP=1.51D-04 DE=-2.24D-06 OVMax= 3.13D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.51D-06 CP: 1.00D+00 1.09D+00 7.48D-01 6.76D-01

E= -1658.67701572793 Delta-E= -0.000000893204 Rises=F Damp=F

DIIS: error= 8.31D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67701572793 IErMin= 5 ErrMin= 8.31D-06

ErrMax= 8.31D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.11D-07 BMatP= 4.15D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.359D-02 0.406D-01 0.147D+00 0.252D+00 0.564D+00

Coeff: -0.359D-02 0.406D-01 0.147D+00 0.252D+00 0.564D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.19D-06 MaxDP=5.62D-05 DE=-8.93D-07 OVMax= 1.52D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 6.94D-07 CP: 1.00D+00 1.09D+00 7.67D-01 7.91D-01 8.19D-01

E= -1658.67701577677 Delta-E= -0.000000048836 Rises=F Damp=F

DIIS: error= 5.07D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67701577677 IErMin= 6 ErrMin= 5.07D-06

ErrMax= 5.07D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.73D-08 BMatP= 2.11D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.246D-03-0.792D-02 0.200D-01 0.567D-01 0.341D+00 0.590D+00

Coeff: 0.246D-03-0.792D-02 0.200D-01 0.567D-01 0.341D+00 0.590D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.64D-07 MaxDP=1.98D-05 DE=-4.88D-08 OVMax= 4.44D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 3.08D-07 CP: 1.00D+00 1.09D+00 7.84D-01 8.01D-01 8.97D-01

CP: 8.75D-01

E= -1658.67701578883 Delta-E= -0.000000012064 Rises=F Damp=F

DIIS: error= 2.00D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67701578883 IErMin= 7 ErrMin= 2.00D-06

ErrMax= 2.00D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.84D-09 BMatP= 4.73D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.549D-03-0.860D-02-0.880D-02-0.856D-02 0.787D-01 0.263D+00

Coeff-Com: 0.684D+00

Coeff: 0.549D-03-0.860D-02-0.880D-02-0.856D-02 0.787D-01 0.263D+00

Coeff: 0.684D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.28D-07 MaxDP=9.29D-06 DE=-1.21D-08 OVMax= 3.45D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.21D-07 CP: 1.00D+00 1.10D+00 7.86D-01 8.21D-01 9.30D-01

CP: 9.98D-01 1.05D+00

E= -1658.67701579013 Delta-E= -0.000000001300 Rises=F Damp=F

DIIS: error= 1.00D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67701579013 IErMin= 8 ErrMin= 1.00D-06

ErrMax= 1.00D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.49D-10 BMatP= 3.84D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.184D-03-0.216D-02-0.627D-02-0.132D-01-0.208D-01 0.124D-01

Coeff-Com: 0.311D+00 0.719D+00

Coeff: 0.184D-03-0.216D-02-0.627D-02-0.132D-01-0.208D-01 0.124D-01

Coeff: 0.311D+00 0.719D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.14D-07 MaxDP=4.56D-06 DE=-1.30D-09 OVMax= 1.72D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 4.84D-08 CP: 1.00D+00 1.10D+00 7.87D-01 8.29D-01 9.44D-01

CP: 1.07D+00 1.22D+00 1.05D+00

E= -1658.67701579043 Delta-E= -0.000000000293 Rises=F Damp=F

DIIS: error= 6.58D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67701579043 IErMin= 9 ErrMin= 6.58D-07

ErrMax= 6.58D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.02D-10 BMatP= 7.49D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.101D-04 0.615D-03-0.176D-02-0.605D-02-0.287D-01-0.507D-01

Coeff-Com: 0.248D-01 0.391D+00 0.671D+00

Coeff: -0.101D-04 0.615D-03-0.176D-02-0.605D-02-0.287D-01-0.507D-01

Coeff: 0.248D-01 0.391D+00 0.671D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.08D-08 MaxDP=2.29D-06 DE=-2.93D-10 OVMax= 5.94D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 2.37D-08 CP: 1.00D+00 1.10D+00 7.88D-01 8.32D-01 9.49D-01

CP: 1.10D+00 1.30D+00 1.17D+00 9.45D-01

E= -1658.67701579047 Delta-E= -0.000000000042 Rises=F Damp=F

DIIS: error= 4.26D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67701579047 IErMin=10 ErrMin= 4.26D-07

ErrMax= 4.26D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.38D-11 BMatP= 2.02D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.468D-04 0.892D-03 0.238D-03-0.103D-02-0.144D-01-0.370D-01

Coeff-Com: -0.580D-01 0.973D-01 0.472D+00 0.540D+00

Coeff: -0.468D-04 0.892D-03 0.238D-03-0.103D-02-0.144D-01-0.370D-01

Coeff: -0.580D-01 0.973D-01 0.472D+00 0.540D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.34D-08 MaxDP=9.00D-07 DE=-4.23D-11 OVMax= 3.20D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.11D-08 CP: 1.00D+00 1.10D+00 7.88D-01 8.33D-01 9.49D-01

CP: 1.11D+00 1.33D+00 1.26D+00 1.07D+00 7.63D-01

E= -1658.67701579050 Delta-E= -0.000000000035 Rises=F Damp=F

DIIS: error= 8.00D-08 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1658.67701579050 IErMin=11 ErrMin= 8.00D-08

ErrMax= 8.00D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.81D-12 BMatP= 8.38D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.140D-04 0.188D-03 0.359D-03 0.702D-03 0.220D-03-0.281D-02

Coeff-Com: -0.230D-01-0.298D-01 0.485D-01 0.178D+00 0.828D+00

Coeff: -0.140D-04 0.188D-03 0.359D-03 0.702D-03 0.220D-03-0.281D-02

Coeff: -0.230D-01-0.298D-01 0.485D-01 0.178D+00 0.828D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=8.09D-09 MaxDP=3.58D-07 DE=-3.46D-11 OVMax= 9.39D-07

Error on total polarization charges = 0.04162

SCF Done: E(UB3LYP) = -1658.67701579 A.U. after 11 cycles

NFock= 11 Conv=0.81D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655236278765D+03 PE=-6.147298581576D+03 EE= 1.731118077091D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.63

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:58:43 2019, MaxMem= 1342177280 cpu: 288.8

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 335

Leave Link 701 at Sat Aug 17 17:58:44 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:58:44 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:58:47 2019, MaxMem= 1342177280 cpu: 38.6

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.41187348D+00-2.95520896D+00 6.29170084D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000150295 -0.000079745 0.000100716

2 6 -0.000101812 0.000012727 -0.000046823

3 8 -0.000139267 0.000089126 -0.000050056

4 8 0.000064885 0.000150848 -0.000015811

5 6 -0.000081090 -0.000050781 0.000047918

6 16 0.000167226 0.000021781 0.000064572

7 6 -0.000069527 0.000025878 -0.000035860

8 16 -0.000142621 0.000022449 -0.000064481

9 16 -0.000023467 -0.000104846 0.000042145

10 6 0.000012985 -0.000002242 0.000044818

11 6 0.000004423 0.000041503 0.000010225

12 6 -0.000021017 0.000017588 0.000053408

13 6 0.000107273 -0.000041247 -0.000036718

14 1 -0.000044746 0.000046150 0.000083790

15 1 -0.000019201 -0.000010934 -0.000048599

16 1 0.000076281 -0.000046375 -0.000001207

17 1 0.000019632 -0.000056842 0.000000334

18 1 0.000016639 -0.000112426 -0.000055782

19 1 -0.000003206 0.000005071 0.000051775

20 1 0.000053366 0.000001594 0.000022525

21 1 0.000051425 -0.000020347 -0.000059405

22 1 -0.000024733 0.000052427 -0.000037933

23 1 0.000017689 0.000000119 0.000044488

24 1 -0.000033290 -0.000000944 0.000035012

25 1 0.000005265 0.000011484 -0.000056378

26 1 -0.000016332 0.000026691 -0.000040569

27 1 -0.000027078 0.000001290 -0.000052103

-------------------------------------------------------------------

Cartesian Forces: Max 0.000167226 RMS 0.000060180

Leave Link 716 at Sat Aug 17 17:58:47 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000161627 RMS 0.000043895

Search for a local minimum.

Step number 62 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .43895D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43 45 44 47 46

49 48 51 50 53

54 55 56 52 57

59 60 61 62

DE= -1.50D-05 DEPred=-1.74D-05 R= 8.62D-01

TightC=F SS= 1.41D+00 RLast= 6.57D-02 DXNew= 8.4625D-02 1.9720D-01

Trust test= 8.62D-01 RLast= 6.57D-02 DXMaxT set to 8.46D-02

ITU= 1 -1 1 0 -1 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1

ITU= 1 1 1 -1 -1 0 -1 -1 -1 0 -1 0 0 -1 -1 0 0 -1 0 0

ITU= -1 1 -1 1 -1 1 1 -1 1 -1 1 1 -1 0 0 -1 0 0 -1 -1

ITU= 0 0

Eigenvalues --- 0.00054 0.00141 0.00170 0.00257 0.00263

Eigenvalues --- 0.00330 0.00399 0.00809 0.01609 0.01901

Eigenvalues --- 0.02744 0.03260 0.03587 0.03863 0.04149

Eigenvalues --- 0.04568 0.04814 0.04925 0.05016 0.05297

Eigenvalues --- 0.05427 0.05462 0.05630 0.05930 0.07875

Eigenvalues --- 0.08128 0.08310 0.10429 0.10934 0.11393

Eigenvalues --- 0.12180 0.12873 0.13445 0.14763 0.15453

Eigenvalues --- 0.15828 0.16108 0.16229 0.16621 0.17158

Eigenvalues --- 0.17969 0.18902 0.20682 0.21816 0.22228

Eigenvalues --- 0.22574 0.23289 0.24736 0.25798 0.27306

Eigenvalues --- 0.27691 0.28871 0.28933 0.29497 0.29765

Eigenvalues --- 0.30686 0.31760 0.33657 0.33776 0.33873

Eigenvalues --- 0.33914 0.33973 0.34043 0.34095 0.34112

Eigenvalues --- 0.34130 0.34170 0.34435 0.34686 0.35460

Eigenvalues --- 0.36907 0.37057 0.49126 0.53023 0.90982

En-DIIS/RFO-DIIS IScMMF= 0 using points: 62 61 60 59

RFO step: Lambda=-8.87742133D-07.

NNeg= 0 NP= 4 Switch= 2.50D-03 Rises=F DC= 2.86D-05 SmlDif= 1.00D-05

RMS Error= 0.3227204381D-03 NUsed= 4 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.22702 0.05029 0.05691 0.66577

Iteration 1 RMS(Cart)= 0.00387948 RMS(Int)= 0.00000828

Iteration 2 RMS(Cart)= 0.00001077 RMS(Int)= 0.00000021

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000021

ITry= 1 IFail=0 DXMaxC= 1.20D-02 DCOld= 1.00D+10 DXMaxT= 8.46D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83596 -0.00008 -0.00035 0.00002 -0.00032 2.83564

R2 2.28912 0.00016 0.00000 0.00008 0.00008 2.28920

R3 2.55346 -0.00010 -0.00040 0.00024 -0.00016 2.55330

R4 2.86494 0.00010 0.00013 0.00018 0.00031 2.86525

R5 3.60995 0.00007 0.00076 -0.00007 0.00069 3.61064

R6 2.05784 0.00008 0.00016 0.00001 0.00017 2.05800

R7 1.83686 0.00003 0.00002 0.00004 0.00006 1.83692

R8 2.06110 0.00006 0.00016 -0.00001 0.00015 2.06125

R9 2.06865 0.00000 0.00001 0.00003 0.00004 2.06870

R10 2.05982 0.00009 0.00014 0.00014 0.00028 2.06010

R11 3.31601 -0.00014 -0.00080 0.00006 -0.00074 3.31526

R12 3.38781 -0.00003 0.00014 0.00006 0.00020 3.38801

R13 3.25404 -0.00009 -0.00007 -0.00023 -0.00030 3.25374

R14 3.47183 0.00012 0.00016 0.00014 0.00030 3.47213

R15 2.88135 0.00003 0.00004 0.00008 0.00012 2.88148

R16 2.06439 -0.00003 -0.00012 0.00002 -0.00010 2.06430

R17 2.06005 0.00001 -0.00002 0.00005 0.00003 2.06008

R18 2.89408 0.00002 0.00004 0.00004 0.00008 2.89416

R19 2.07224 -0.00002 -0.00004 -0.00001 -0.00005 2.07219

R20 2.07122 -0.00001 -0.00007 0.00003 -0.00004 2.07118

R21 2.88600 0.00008 0.00010 0.00011 0.00022 2.88622

R22 2.07203 -0.00003 -0.00009 0.00001 -0.00008 2.07195

R23 2.07176 0.00002 0.00002 0.00003 0.00006 2.07181

R24 2.06764 0.00001 0.00000 0.00003 0.00002 2.06766

R25 2.06934 -0.00002 -0.00008 0.00000 -0.00008 2.06926

R26 2.06897 0.00003 0.00006 0.00004 0.00010 2.06907

A1 2.17599 0.00012 0.00024 0.00032 0.00056 2.17655

A2 1.97736 -0.00014 0.00011 -0.00044 -0.00033 1.97703

A3 2.12926 0.00002 -0.00036 0.00012 -0.00024 2.12902

A4 2.02683 -0.00005 0.00037 -0.00076 -0.00039 2.02644

A5 1.83039 0.00003 -0.00051 0.00084 0.00032 1.83072

A6 1.87297 0.00001 0.00030 0.00010 0.00040 1.87337

A7 1.94726 -0.00004 -0.00062 -0.00027 -0.00089 1.94637

A8 1.94101 0.00002 0.00041 0.00015 0.00057 1.94158

A9 1.83193 0.00002 -0.00001 0.00004 0.00004 1.83197

A10 1.87224 0.00006 0.00003 0.00049 0.00051 1.87275

A11 1.91294 0.00000 -0.00006 -0.00004 -0.00010 1.91284

A12 1.92601 0.00002 0.00033 0.00019 0.00053 1.92654

A13 1.95237 0.00001 -0.00005 -0.00005 -0.00011 1.95226

A14 1.88345 0.00000 -0.00002 0.00005 0.00003 1.88349

A15 1.89455 -0.00002 -0.00030 -0.00019 -0.00049 1.89405

A16 1.89293 -0.00001 0.00009 0.00004 0.00013 1.89306

A17 1.79834 -0.00003 0.00018 0.00015 0.00033 1.79867

A18 1.97017 0.00002 -0.00018 -0.00082 -0.00100 1.96917

A19 2.14283 -0.00003 0.00017 0.00039 0.00056 2.14339

A20 2.15521 0.00000 -0.00003 0.00041 0.00038 2.15559

A21 1.79595 0.00006 -0.00014 0.00056 0.00041 1.79636

A22 1.92572 0.00009 0.00073 0.00005 0.00078 1.92650

A23 1.88018 -0.00005 -0.00080 0.00034 -0.00046 1.87972

A24 1.89109 0.00003 0.00064 -0.00005 0.00059 1.89168

A25 1.93955 -0.00003 -0.00007 -0.00017 -0.00024 1.93930

A26 1.93834 -0.00004 -0.00022 -0.00003 -0.00025 1.93809

A27 1.88709 0.00001 -0.00031 -0.00012 -0.00043 1.88667

A28 1.95304 0.00004 -0.00018 0.00012 -0.00006 1.95298

A29 1.91537 0.00003 0.00046 0.00013 0.00060 1.91597

A30 1.91755 -0.00004 -0.00018 -0.00008 -0.00026 1.91729

A31 1.90699 -0.00004 -0.00007 -0.00005 -0.00012 1.90687

A32 1.90867 0.00000 -0.00019 -0.00006 -0.00026 1.90841

A33 1.85984 0.00001 0.00019 -0.00008 0.00011 1.85995

A34 1.96593 0.00002 0.00013 0.00008 0.00021 1.96613

A35 1.90652 -0.00001 -0.00032 0.00011 -0.00021 1.90632

A36 1.90772 -0.00001 0.00009 -0.00017 -0.00007 1.90765

A37 1.91312 -0.00002 -0.00016 -0.00006 -0.00022 1.91290

A38 1.91245 0.00002 0.00020 0.00011 0.00032 1.91277

A39 1.85477 0.00000 0.00004 -0.00008 -0.00004 1.85474

A40 1.94543 0.00001 -0.00001 0.00004 0.00003 1.94546

A41 1.94230 -0.00005 -0.00021 0.00000 -0.00021 1.94208

A42 1.94290 -0.00001 0.00004 -0.00005 -0.00001 1.94289

A43 1.87680 0.00002 0.00012 0.00004 0.00015 1.87695

A44 1.87717 0.00000 0.00007 -0.00009 -0.00002 1.87715

A45 1.87585 0.00002 0.00001 0.00007 0.00008 1.87593

D1 2.70131 0.00002 0.00763 -0.00757 0.00006 2.70137

D2 -1.42397 -0.00004 0.00668 -0.00777 -0.00109 -1.42506

D3 0.51787 0.00001 0.00657 -0.00731 -0.00074 0.51713

D4 -0.47595 0.00001 0.00744 -0.00781 -0.00038 -0.47633

D5 1.68195 -0.00004 0.00649 -0.00801 -0.00152 1.68042

D6 -2.65939 0.00000 0.00638 -0.00756 -0.00118 -2.66057

D7 -3.10063 0.00001 0.00104 -0.00011 0.00092 -3.09971

D8 0.00637 0.00000 0.00086 -0.00034 0.00052 0.00689

D9 -3.13813 -0.00003 -0.00425 -0.00126 -0.00551 3.13954

D10 -1.06626 -0.00002 -0.00410 -0.00111 -0.00521 -1.07147

D11 1.04283 -0.00001 -0.00379 -0.00097 -0.00476 1.03808

D12 1.04910 -0.00001 -0.00335 -0.00161 -0.00495 1.04415

D13 3.12097 0.00000 -0.00320 -0.00145 -0.00465 3.11632

D14 -1.05312 0.00001 -0.00289 -0.00131 -0.00420 -1.05732

D15 -0.98983 -0.00003 -0.00321 -0.00158 -0.00479 -0.99462

D16 1.08204 -0.00002 -0.00307 -0.00143 -0.00449 1.07754

D17 -3.09205 -0.00001 -0.00275 -0.00129 -0.00404 -3.09609

D18 -3.08689 0.00003 -0.00092 -0.00051 -0.00143 -3.08832

D19 -0.87887 -0.00003 -0.00120 -0.00104 -0.00224 -0.88111

D20 1.22520 -0.00001 -0.00104 -0.00098 -0.00202 1.22319

D21 1.82000 0.00000 0.00112 0.00051 0.00163 1.82163

D22 -1.14223 0.00006 0.00136 0.00055 0.00191 -1.14033

D23 2.59017 0.00006 0.00336 0.00212 0.00548 2.59565

D24 -0.73226 -0.00001 0.00315 0.00207 0.00522 -0.72704

D25 -3.03638 0.00002 0.00357 -0.00278 0.00079 -3.03559

D26 -0.91634 0.00000 0.00342 -0.00275 0.00067 -0.91567

D27 1.12131 0.00000 0.00297 -0.00274 0.00023 1.12155

D28 -3.12235 -0.00004 -0.00064 -0.00098 -0.00162 -3.12397

D29 -1.00231 -0.00004 -0.00053 -0.00087 -0.00140 -1.00371

D30 1.03715 -0.00003 -0.00014 -0.00093 -0.00107 1.03608

D31 1.07642 -0.00001 -0.00007 -0.00133 -0.00140 1.07502

D32 -3.08672 -0.00001 0.00003 -0.00121 -0.00118 -3.08790

D33 -1.04727 -0.00001 0.00043 -0.00127 -0.00084 -1.04811

D34 -1.02506 0.00002 0.00052 -0.00104 -0.00052 -1.02558

D35 1.09498 0.00002 0.00062 -0.00093 -0.00031 1.09468

D36 3.13444 0.00003 0.00101 -0.00098 0.00003 3.13447

D37 -3.13153 0.00004 -0.00056 -0.00096 -0.00151 -3.13304

D38 -1.00126 0.00001 -0.00090 -0.00091 -0.00181 -1.00307

D39 1.02140 0.00001 -0.00097 -0.00104 -0.00201 1.01940

D40 1.02679 0.00000 -0.00097 -0.00117 -0.00214 1.02465

D41 -3.12612 -0.00003 -0.00131 -0.00113 -0.00244 -3.12856

D42 -1.10346 -0.00004 -0.00138 -0.00125 -0.00264 -1.10610

D43 -1.00274 0.00001 -0.00105 -0.00102 -0.00206 -1.00481

D44 1.12753 -0.00001 -0.00139 -0.00097 -0.00236 1.12517

D45 -3.13300 -0.00002 -0.00146 -0.00110 -0.00256 -3.13556

D46 -3.13835 -0.00003 -0.00747 0.00062 -0.00685 3.13799

D47 -1.04328 -0.00003 -0.00747 0.00069 -0.00678 -1.05005

D48 1.04889 -0.00004 -0.00758 0.00075 -0.00683 1.04205

D49 1.01830 -0.00001 -0.00704 0.00047 -0.00657 1.01174

D50 3.11337 -0.00001 -0.00704 0.00055 -0.00649 3.10688

D51 -1.07765 -0.00002 -0.00715 0.00060 -0.00655 -1.08420

D52 -1.01077 -0.00002 -0.00712 0.00054 -0.00658 -1.01734

D53 1.08431 -0.00001 -0.00712 0.00061 -0.00650 1.07780

D54 -3.10672 -0.00002 -0.00723 0.00067 -0.00656 -3.11328

Item Value Threshold Converged?

Maximum Force 0.000162 0.000450 YES

RMS Force 0.000044 0.000300 YES

Maximum Displacement 0.012034 0.001800 NO

RMS Displacement 0.003878 0.001200 NO

Predicted change in Energy=-2.357800D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:58:48 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.096957 -0.405682 -0.199166

2 6 0 -2.844359 0.074106 0.473494

3 8 0 -4.900919 0.311873 -0.752542

4 8 0 -4.235985 -1.749402 -0.172883

5 6 0 -2.295657 -0.813690 1.573353

6 16 0 -1.581207 0.297435 -0.942564

7 6 0 -0.117886 0.769173 -0.097614

8 16 0 1.081221 -0.559209 0.011400

9 16 0 0.022179 2.249663 0.770228

10 6 0 2.686808 0.333908 -0.007933

11 6 0 3.844538 -0.656327 -0.072324

12 6 0 5.202651 0.051516 -0.065088

13 6 0 6.375022 -0.924430 -0.141175

14 1 0 -3.037860 1.081502 0.839191

15 1 0 -5.048177 -1.965599 -0.661240

16 1 0 -1.389096 -0.368214 1.985022

17 1 0 -3.023323 -0.908145 2.385735

18 1 0 -2.055463 -1.812017 1.207164

19 1 0 2.687516 0.997109 -0.875951

20 1 0 2.748262 0.950214 0.889177

21 1 0 3.791280 -1.345284 0.779104

22 1 0 3.759721 -1.269843 -0.976571

23 1 0 5.250190 0.750026 -0.908874

24 1 0 5.289240 0.660125 0.842709

25 1 0 7.334555 -0.398625 -0.138408

26 1 0 6.373970 -1.613761 0.709622

27 1 0 6.331896 -1.528058 -1.053641

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.500557 0.000000

3 O 1.211391 2.406063 0.000000

4 O 1.351149 2.383193 2.242097 0.000000

5 C 2.559877 1.516226 3.669342 2.773043 0.000000

6 S 2.715881 1.910667 3.325177 3.439447 2.841632

7 C 4.150133 2.871052 4.849274 4.827797 3.168639

8 S 5.184730 4.003098 6.093307 5.451898 3.729311

9 S 4.995785 3.610837 5.505521 5.917258 3.924476

10 C 6.826641 5.558154 7.624207 7.231352 5.351860

11 C 7.946462 6.750763 8.825142 8.154740 6.358854

12 C 9.311805 8.065045 10.130277 9.609514 7.723839

13 C 10.484979 9.293647 11.359976 10.643075 8.839261

14 H 2.100378 1.089047 2.568450 3.236327 2.163703

15 H 1.884588 3.210114 2.284054 0.972055 3.727823

16 H 3.479165 2.144330 4.504407 3.830015 1.090768

17 H 2.843742 2.157199 3.855204 2.953775 1.094707

18 H 2.850130 2.172115 4.055611 2.581303 1.090158

19 H 6.960958 5.768412 7.620310 7.481476 5.840385

20 H 7.062575 5.676070 7.849375 7.562777 5.387075

21 H 8.004008 6.792626 8.980336 8.093613 6.161512

22 H 7.942199 6.893675 8.806742 8.050292 6.586182

23 H 9.445025 8.239510 10.161763 9.837496 8.096077

24 H 9.503796 8.163036 10.320148 9.877609 7.761227

25 H 11.431676 10.208241 12.271463 11.649171 9.789964

26 H 10.579493 9.374553 11.531224 10.647458 8.749205

27 H 10.523822 9.439424 11.386490 10.606830 9.046883

6 7 8 9 10

6 S 0.000000

7 C 1.754362 0.000000

8 S 2.955065 1.792858 0.000000

9 S 3.052163 1.721807 3.096313 0.000000

10 C 4.369305 2.839685 1.837374 3.372818 0.000000

11 C 5.577248 4.211116 2.766291 4.874946 1.524812

12 C 6.844792 5.368818 4.167136 5.689190 2.532287

13 C 8.089299 6.710294 5.308577 7.159897 3.899242

14 H 2.431306 3.082434 4.510432 3.276156 5.835096

15 H 4.149741 5.666076 6.324547 6.747299 8.095959

16 H 3.008447 2.692025 3.167669 3.212585 4.591061

17 H 3.822393 4.173965 4.754629 4.675115 6.314898

18 H 3.048940 3.481263 3.583038 4.583094 5.345146

19 H 4.326197 2.920281 2.406180 3.373843 1.092378

20 H 4.746125 3.036666 2.414100 3.022291 1.090145

21 H 5.875908 4.530027 2.924330 5.208632 2.158465

22 H 5.566241 4.468332 2.942015 5.422863 2.159032

23 H 6.846456 5.429065 4.465569 5.692134 2.748777

24 H 7.107868 5.489363 4.459291 5.502164 2.757292

25 H 8.978975 7.543494 6.257190 7.830063 4.706929

26 H 8.346691 6.962342 5.441764 7.434714 4.231248

27 H 8.121697 6.913100 5.444499 7.576952 4.224581

11 12 13 14 15

11 C 0.000000

12 C 1.531523 0.000000

13 C 2.545577 1.527323 0.000000

14 H 7.156697 8.353718 9.674049 0.000000

15 H 9.007853 10.464398 11.482333 3.946833 0.000000

16 H 5.630862 6.915942 8.069177 2.476495 4.789908

17 H 7.298835 8.636789 9.732133 2.520060 3.808188

18 H 6.146765 7.600762 8.583641 3.077817 3.531411

19 H 2.172180 2.806697 4.222547 5.977354 8.286416

20 H 2.169627 2.782499 4.210618 5.787827 8.467008

21 H 1.096553 2.157702 2.774843 7.247762 8.977494

22 H 1.096019 2.158434 2.767127 7.418418 8.840961

23 H 2.157197 1.096427 2.158335 8.476873 10.653277

24 H 2.158123 1.096356 2.158186 8.337755 10.771188

25 H 3.500142 2.180142 1.094159 10.522997 12.492431

26 H 2.815341 2.178374 1.095004 9.791005 11.509497

27 H 2.812445 2.178872 1.094906 9.908831 11.395240

16 17 18 19 20

16 H 0.000000

17 H 1.767143 0.000000

18 H 1.770219 1.772785 0.000000

19 H 5.164110 6.847063 5.892911 0.000000

20 H 4.478488 6.245348 5.550388 1.766795 0.000000

21 H 5.407883 7.015067 5.880942 3.073159 2.523750

22 H 6.007852 7.579288 6.235304 2.509745 3.071273

23 H 7.328384 9.058421 8.025848 2.574768 3.087508

24 H 6.852921 8.598785 7.758155 3.136290 2.557905

25 H 8.978417 10.673170 9.590656 4.907853 4.889722

26 H 7.965126 9.571644 8.446431 4.787549 4.444318

27 H 8.378092 9.986677 8.691355 4.437290 4.770619

21 22 23 24 25

21 H 0.000000

22 H 1.757578 0.000000

23 H 3.060721 2.511165 0.000000

24 H 2.503916 3.061696 1.754323 0.000000

25 H 3.780581 3.773722 2.501519 2.503369 0.000000

26 H 2.597537 3.129828 3.077320 2.522877 1.765908

27 H 3.138007 2.586252 2.526006 3.077567 1.765954

26 27

26 H 0.000000

27 H 1.765846 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 2.37D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.104937 -0.464423 -0.124623

2 6 0 -2.847323 0.117533 0.451054

3 8 0 -4.912871 0.153698 -0.782374

4 8 0 -4.243962 -1.785428 0.122807

5 6 0 -2.290622 -0.578505 1.677658

6 16 0 -1.594659 0.103766 -0.991614

7 6 0 -0.125053 0.705764 -0.246202

8 16 0 1.074635 -0.588354 0.070576

9 16 0 0.021651 2.308396 0.365900

10 6 0 2.680166 0.287304 -0.106735

11 6 0 3.837243 -0.701648 -0.016193

12 6 0 5.195475 -0.004057 -0.135092

13 6 0 6.367108 -0.980852 -0.058539

14 1 0 -3.037964 1.171542 0.647889

15 1 0 -5.059780 -2.077722 -0.317529

16 1 0 -1.380972 -0.072750 2.004038

17 1 0 -3.012266 -0.537392 2.499804

18 1 0 -2.053290 -1.623712 1.478510

19 1 0 2.674542 0.799086 -1.071794

20 1 0 2.748350 1.042374 0.676614

21 1 0 3.790190 -1.241488 0.937111

22 1 0 3.745643 -1.455105 -0.806869

23 1 0 5.236866 0.546468 -1.082384

24 1 0 5.288872 0.745141 0.659878

25 1 0 7.326712 -0.463024 -0.149074

26 1 0 6.372256 -1.521235 0.893824

27 1 0 6.317139 -1.725961 -0.859248

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3049853 0.1934424 0.1808388

Leave Link 202 at Sat Aug 17 17:58:48 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.3029518873 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0549975336 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.2479543537 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

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Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2321

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.57D-10

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 97

GePol: Fraction of low-weight points (<1% of avg) = 4.18%

GePol: Cavity surface area = 309.276 Ang\*\*2

GePol: Cavity volume = 320.436 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057869047 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.2421674491 Hartrees.

Leave Link 301 at Sat Aug 17 17:58:48 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:58:48 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:58:48 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000474 -0.000032 0.000021 Ang= -0.05 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 17:58:48 2019, MaxMem= 1342177280 cpu: 2.7

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16161123.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.33D-15 for 2310.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.84D-15 for 2273 1692.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.77D-15 for 2310.

Iteration 1 A^-1\*A deviation from orthogonality is 2.57D-10 for 2130 896.

Iteration 2 A\*A^-1 deviation from unit magnitude is 3.66D-15 for 1624.

Iteration 2 A\*A^-1 deviation from orthogonality is 2.67D-15 for 796 684.

Iteration 2 A^-1\*A deviation from unit magnitude is 9.99D-16 for 226.

Iteration 2 A^-1\*A deviation from orthogonality is 6.86D-16 for 2293 175.

E= -1658.67698734430

DIIS: error= 1.90D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67698734430 IErMin= 1 ErrMin= 1.90D-04

ErrMax= 1.90D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.91D-05 BMatP= 6.91D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.90D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.428 Goal= None Shift= 0.000

Gap= 0.484 Goal= None Shift= 0.000

RMSDP=2.16D-05 MaxDP=9.84D-04 OVMax= 1.48D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.16D-05 CP: 1.00D+00

E= -1658.67702125097 Delta-E= -0.000033906670 Rises=F Damp=F

DIIS: error= 2.50D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67702125097 IErMin= 2 ErrMin= 2.50D-05

ErrMax= 2.50D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.20D-06 BMatP= 6.91D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.647D-01 0.106D+01

Coeff: -0.647D-01 0.106D+01

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.48D-06 MaxDP=1.34D-04 DE=-3.39D-05 OVMax= 4.32D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 4.27D-06 CP: 1.00D+00 1.06D+00

E= -1658.67702151314 Delta-E= -0.000000262174 Rises=F Damp=F

DIIS: error= 3.07D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67702151314 IErMin= 2 ErrMin= 2.50D-05

ErrMax= 3.07D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.13D-06 BMatP= 1.20D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.427D-01 0.566D+00 0.477D+00

Coeff: -0.427D-01 0.566D+00 0.477D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.37D-06 MaxDP=9.96D-05 DE=-2.62D-07 OVMax= 2.07D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.65D-06 CP: 1.00D+00 1.10D+00 6.38D-01

E= -1658.67702173920 Delta-E= -0.000000226064 Rises=F Damp=F

DIIS: error= 1.60D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67702173920 IErMin= 4 ErrMin= 1.60D-05

ErrMax= 1.60D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.27D-07 BMatP= 1.13D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.158D-01 0.187D+00 0.313D+00 0.515D+00

Coeff: -0.158D-01 0.187D+00 0.313D+00 0.515D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=9.09D-07 MaxDP=3.80D-05 DE=-2.26D-07 OVMax= 9.76D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 6.63D-07 CP: 1.00D+00 1.11D+00 7.13D-01 7.25D-01

E= -1658.67702179175 Delta-E= -0.000000052548 Rises=F Damp=F

DIIS: error= 2.19D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67702179175 IErMin= 5 ErrMin= 2.19D-06

ErrMax= 2.19D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.54D-09 BMatP= 2.27D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.214D-02 0.169D-01 0.839D-01 0.222D+00 0.680D+00

Coeff: -0.214D-02 0.169D-01 0.839D-01 0.222D+00 0.680D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.54D-07 MaxDP=9.75D-06 DE=-5.25D-08 OVMax= 2.17D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.75D-07 CP: 1.00D+00 1.11D+00 7.45D-01 7.95D-01 9.77D-01

E= -1658.67702179395 Delta-E= -0.000000002202 Rises=F Damp=F

DIIS: error= 7.77D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67702179395 IErMin= 6 ErrMin= 7.77D-07

ErrMax= 7.77D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.66D-09 BMatP= 8.54D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.111D-02-0.187D-01 0.430D-03 0.508D-01 0.350D+00 0.616D+00

Coeff: 0.111D-02-0.187D-01 0.430D-03 0.508D-01 0.350D+00 0.616D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.27D-07 MaxDP=4.67D-06 DE=-2.20D-09 OVMax= 1.60D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 8.06D-08 CP: 1.00D+00 1.11D+00 7.58D-01 8.33D-01 1.05D+00

CP: 9.00D-01

E= -1658.67702179452 Delta-E= -0.000000000563 Rises=F Damp=F

DIIS: error= 5.27D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67702179452 IErMin= 7 ErrMin= 5.27D-07

ErrMax= 5.27D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.16D-10 BMatP= 1.66D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.721D-03-0.954D-02-0.115D-01-0.808D-02 0.336D-01 0.263D+00

Coeff-Com: 0.732D+00

Coeff: 0.721D-03-0.954D-02-0.115D-01-0.808D-02 0.336D-01 0.263D+00

Coeff: 0.732D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.58D-08 MaxDP=2.87D-06 DE=-5.63D-10 OVMax= 9.43D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 3.22D-08 CP: 1.00D+00 1.11D+00 7.64D-01 8.40D-01 1.10D+00

CP: 1.05D+00 1.18D+00

E= -1658.67702179457 Delta-E= -0.000000000050 Rises=F Damp=F

DIIS: error= 3.47D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67702179457 IErMin= 8 ErrMin= 3.47D-07

ErrMax= 3.47D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.32D-10 BMatP= 2.16D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.245D-03-0.210D-02-0.872D-02-0.185D-01-0.677D-01 0.355D-01

Coeff-Com: 0.524D+00 0.538D+00

Coeff: 0.245D-03-0.210D-02-0.872D-02-0.185D-01-0.677D-01 0.355D-01

Coeff: 0.524D+00 0.538D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.04D-08 MaxDP=1.30D-06 DE=-5.00D-11 OVMax= 2.90D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.35D-08 CP: 1.00D+00 1.11D+00 7.66D-01 8.49D-01 1.12D+00

CP: 1.13D+00 1.32D+00 7.48D-01

E= -1658.67702179460 Delta-E= -0.000000000030 Rises=F Damp=F

DIIS: error= 9.09D-08 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67702179460 IErMin= 9 ErrMin= 9.09D-08

ErrMax= 9.09D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.81D-12 BMatP= 1.32D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.458D-04 0.122D-02-0.164D-02-0.650D-02-0.392D-01-0.373D-01

Coeff-Com: 0.909D-01 0.247D+00 0.746D+00

Coeff: -0.458D-04 0.122D-02-0.164D-02-0.650D-02-0.392D-01-0.373D-01

Coeff: 0.909D-01 0.247D+00 0.746D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.33D-08 MaxDP=5.22D-07 DE=-3.00D-11 OVMax= 1.91D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 5.01D-09 CP: 1.00D+00 1.11D+00 7.67D-01 8.50D-01 1.13D+00

CP: 1.16D+00 1.40D+00 8.87D-01 8.86D-01

E= -1658.67702179462 Delta-E= -0.000000000024 Rises=F Damp=F

DIIS: error= 2.53D-08 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67702179462 IErMin=10 ErrMin= 2.53D-08

ErrMax= 2.53D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.35D-12 BMatP= 8.81D-12

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.432D-04 0.760D-03-0.667D-04-0.140D-02-0.124D-01-0.213D-01

Coeff-Com: -0.605D-02 0.619D-01 0.362D+00 0.617D+00

Coeff: -0.432D-04 0.760D-03-0.667D-04-0.140D-02-0.124D-01-0.213D-01

Coeff: -0.605D-02 0.619D-01 0.362D+00 0.617D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.81D-09 MaxDP=9.64D-08 DE=-2.36D-11 OVMax= 2.89D-07

Error on total polarization charges = 0.04162

SCF Done: E(UB3LYP) = -1658.67702179 A.U. after 10 cycles

NFock= 10 Conv=0.28D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655235708480D+03 PE=-6.147247740185D+03 EE= 1.731092842461D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.63

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:59:11 2019, MaxMem= 1342177280 cpu: 259.8

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 336

Leave Link 701 at Sat Aug 17 17:59:12 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:59:12 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:59:15 2019, MaxMem= 1342177280 cpu: 38.3

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.41585907D+00-2.95369235D+00 6.31098237D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000059811 -0.000075269 -0.000017321

2 6 -0.000001170 -0.000046885 0.000057395

3 8 -0.000088959 0.000147525 -0.000006227

4 8 0.000034884 -0.000015175 -0.000023763

5 6 0.000019442 -0.000039977 0.000025274

6 16 0.000008561 0.000067420 -0.000024952

7 6 0.000003350 -0.000004466 -0.000012341

8 16 0.000015935 -0.000011746 0.000017246

9 16 -0.000016527 -0.000050797 0.000062309

10 6 0.000018676 0.000037369 0.000044945

11 6 -0.000010663 0.000002845 -0.000036017

12 6 -0.000016830 0.000038137 0.000008071

13 6 0.000019206 -0.000012172 -0.000016702

14 1 -0.000010429 -0.000020902 0.000066780

15 1 0.000003638 0.000048659 -0.000021005

16 1 0.000006716 -0.000035241 0.000021286

17 1 0.000007667 -0.000051122 -0.000028777

18 1 -0.000014019 -0.000008039 -0.000034989

19 1 0.000011770 0.000021670 0.000011852

20 1 -0.000020651 -0.000029603 0.000043822

21 1 -0.000000975 -0.000011445 -0.000037156

22 1 -0.000014853 0.000017642 -0.000031699

23 1 0.000001479 0.000020437 0.000020147

24 1 0.000010133 -0.000019811 0.000019338

25 1 -0.000005600 0.000005863 -0.000021121

26 1 -0.000004517 -0.000014984 -0.000046113

27 1 -0.000016076 0.000040067 -0.000040280

-------------------------------------------------------------------

Cartesian Forces: Max 0.000147525 RMS 0.000035075

Leave Link 716 at Sat Aug 17 17:59:15 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000143368 RMS 0.000024746

Search for a local minimum.

Step number 63 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .24746D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43 45 44 47 46

49 48 51 50 53

54 55 56 52 57

59 60 61 62 63

DE= -6.00D-06 DEPred=-2.36D-06 R= 2.55D+00

TightC=F SS= 1.41D+00 RLast= 2.73D-02 DXNew= 1.4232D-01 8.1854D-02

Trust test= 2.55D+00 RLast= 2.73D-02 DXMaxT set to 8.46D-02

ITU= 1 1 -1 1 0 -1 0 0 0 0 0 0 0 0 0 0 0 0 0 1

ITU= 1 1 1 1 -1 -1 0 -1 -1 -1 0 -1 0 0 -1 -1 0 0 -1 0

ITU= 0 -1 1 -1 1 -1 1 1 -1 1 -1 1 1 -1 0 0 -1 0 0 -1

ITU= -1 0 0

Eigenvalues --- 0.00047 0.00080 0.00171 0.00195 0.00298

Eigenvalues --- 0.00318 0.00395 0.00768 0.01286 0.01910

Eigenvalues --- 0.03017 0.03515 0.03689 0.03847 0.04127

Eigenvalues --- 0.04604 0.04681 0.04784 0.04967 0.05377

Eigenvalues --- 0.05479 0.05564 0.05641 0.05872 0.08029

Eigenvalues --- 0.08162 0.08328 0.09539 0.10837 0.11213

Eigenvalues --- 0.11761 0.12096 0.14213 0.15193 0.15684

Eigenvalues --- 0.16006 0.16064 0.16194 0.16570 0.17113

Eigenvalues --- 0.18670 0.19386 0.20333 0.21528 0.22058

Eigenvalues --- 0.22203 0.22848 0.24110 0.25396 0.25897

Eigenvalues --- 0.26979 0.28544 0.28860 0.29339 0.29651

Eigenvalues --- 0.29756 0.30474 0.33209 0.33600 0.33858

Eigenvalues --- 0.33873 0.33929 0.33975 0.34007 0.34099

Eigenvalues --- 0.34115 0.34151 0.34299 0.34959 0.35131

Eigenvalues --- 0.35436 0.38675 0.47218 0.52626 0.91210

En-DIIS/RFO-DIIS IScMMF= 0 using points: 63 62 61 60 59

RFO step: Lambda=-1.55343229D-07.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 2.86D-05 SmlDif= 1.00D-05

RMS Error= 0.1001537421D-03 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.16074 0.06754 0.00509 0.04384 -0.27721

Iteration 1 RMS(Cart)= 0.01169020 RMS(Int)= 0.00005999

Iteration 2 RMS(Cart)= 0.00007507 RMS(Int)= 0.00000016

Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00000016

ITry= 1 IFail=0 DXMaxC= 5.76D-02 DCOld= 1.00D+10 DXMaxT= 8.46D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83564 -0.00001 -0.00007 0.00021 0.00014 2.83578

R2 2.28920 0.00014 -0.00003 -0.00021 -0.00024 2.28895

R3 2.55330 0.00000 0.00001 0.00029 0.00030 2.55360

R4 2.86525 0.00001 0.00004 -0.00025 -0.00021 2.86504

R5 3.61064 0.00004 -0.00039 -0.00045 -0.00084 3.60980

R6 2.05800 0.00000 -0.00009 -0.00022 -0.00030 2.05770

R7 1.83692 -0.00002 -0.00002 -0.00016 -0.00018 1.83674

R8 2.06125 0.00002 -0.00004 0.00001 -0.00003 2.06122

R9 2.06870 -0.00002 0.00000 -0.00024 -0.00024 2.06846

R10 2.06010 -0.00002 -0.00002 0.00001 -0.00001 2.06009

R11 3.31526 -0.00004 0.00025 -0.00027 -0.00003 3.31524

R12 3.38801 -0.00001 -0.00003 0.00059 0.00056 3.38857

R13 3.25374 -0.00004 -0.00001 -0.00049 -0.00050 3.25324

R14 3.47213 -0.00001 -0.00014 0.00010 -0.00004 3.47209

R15 2.88148 -0.00003 0.00000 -0.00036 -0.00036 2.88112

R16 2.06430 0.00001 0.00000 -0.00028 -0.00028 2.06401

R17 2.06008 0.00000 -0.00001 -0.00005 -0.00006 2.06002

R18 2.89416 0.00000 -0.00002 -0.00009 -0.00012 2.89404

R19 2.07219 -0.00001 -0.00001 -0.00017 -0.00018 2.07200

R20 2.07118 0.00001 -0.00002 -0.00021 -0.00023 2.07095

R21 2.88622 0.00000 -0.00003 0.00035 0.00032 2.88654

R22 2.07195 0.00000 0.00000 -0.00028 -0.00028 2.07167

R23 2.07181 0.00000 -0.00002 -0.00011 -0.00013 2.07168

R24 2.06766 0.00000 -0.00002 -0.00017 -0.00019 2.06747

R25 2.06926 0.00000 0.00000 -0.00031 -0.00031 2.06894

R26 2.06907 -0.00001 -0.00002 -0.00013 -0.00016 2.06892

A1 2.17655 -0.00003 0.00009 0.00050 0.00058 2.17714

A2 1.97703 -0.00003 -0.00012 -0.00093 -0.00105 1.97599

A3 2.12902 0.00006 0.00003 0.00044 0.00048 2.12950

A4 2.02644 0.00005 -0.00032 0.00034 0.00002 2.02647

A5 1.83072 -0.00005 0.00050 0.00079 0.00128 1.83200

A6 1.87337 -0.00001 0.00005 -0.00015 -0.00010 1.87327

A7 1.94637 0.00002 0.00001 -0.00039 -0.00038 1.94599

A8 1.94158 -0.00004 -0.00002 0.00029 0.00027 1.94185

A9 1.83197 0.00002 -0.00018 -0.00099 -0.00117 1.83079

A10 1.87275 -0.00003 -0.00003 0.00020 0.00018 1.87293

A11 1.91284 0.00001 0.00002 0.00035 0.00037 1.91321

A12 1.92654 -0.00002 -0.00003 0.00005 0.00003 1.92656

A13 1.95226 -0.00001 0.00002 -0.00055 -0.00053 1.95173

A14 1.88349 0.00000 -0.00004 -0.00013 -0.00017 1.88331

A15 1.89405 0.00001 0.00003 0.00005 0.00008 1.89413

A16 1.89306 0.00001 -0.00001 0.00024 0.00023 1.89329

A17 1.79867 -0.00010 -0.00013 -0.00150 -0.00163 1.79704

A18 1.96917 0.00007 -0.00027 0.00069 0.00042 1.96959

A19 2.14339 -0.00006 0.00008 -0.00018 -0.00010 2.14329

A20 2.15559 -0.00002 0.00010 -0.00029 -0.00019 2.15541

A21 1.79636 -0.00004 0.00007 -0.00092 -0.00085 1.79551

A22 1.92650 -0.00004 -0.00019 -0.00053 -0.00072 1.92578

A23 1.87972 0.00002 0.00025 -0.00073 -0.00048 1.87925

A24 1.89168 0.00000 -0.00006 0.00110 0.00104 1.89272

A25 1.93930 -0.00001 0.00009 -0.00036 -0.00027 1.93903

A26 1.93809 0.00003 -0.00008 0.00017 0.00009 1.93818

A27 1.88667 0.00001 -0.00001 0.00039 0.00037 1.88704

A28 1.95298 0.00001 0.00006 0.00057 0.00063 1.95361

A29 1.91597 0.00000 -0.00011 0.00043 0.00032 1.91629

A30 1.91729 -0.00001 0.00002 -0.00082 -0.00080 1.91649

A31 1.90687 0.00000 0.00003 -0.00032 -0.00029 1.90659

A32 1.90841 0.00000 -0.00001 0.00034 0.00032 1.90874

A33 1.85995 0.00000 0.00001 -0.00024 -0.00022 1.85973

A34 1.96613 -0.00003 0.00000 -0.00067 -0.00067 1.96546

A35 1.90632 0.00001 0.00002 -0.00019 -0.00017 1.90614

A36 1.90765 0.00002 -0.00001 0.00071 0.00070 1.90834

A37 1.91290 0.00001 0.00007 -0.00063 -0.00056 1.91233

A38 1.91277 0.00001 -0.00004 0.00078 0.00073 1.91350

A39 1.85474 0.00000 -0.00002 0.00004 0.00001 1.85475

A40 1.94546 0.00000 -0.00001 0.00025 0.00024 1.94569

A41 1.94208 0.00000 0.00003 0.00014 0.00017 1.94225

A42 1.94289 -0.00002 0.00005 -0.00070 -0.00065 1.94223

A43 1.87695 0.00001 -0.00006 0.00023 0.00017 1.87713

A44 1.87715 0.00001 -0.00003 -0.00019 -0.00021 1.87694

A45 1.87593 0.00001 0.00001 0.00030 0.00031 1.87623

D1 2.70137 -0.00003 -0.00471 -0.00976 -0.01447 2.68690

D2 -1.42506 -0.00001 -0.00452 -0.00943 -0.01396 -1.43902

D3 0.51713 -0.00001 -0.00449 -0.01027 -0.01475 0.50238

D4 -0.47633 -0.00002 -0.00458 -0.00942 -0.01400 -0.49033

D5 1.68042 0.00000 -0.00440 -0.00909 -0.01349 1.66693

D6 -2.66057 0.00000 -0.00436 -0.00993 -0.01429 -2.67486

D7 -3.09971 -0.00002 0.00005 -0.00266 -0.00261 -3.10232

D8 0.00689 0.00000 0.00017 -0.00233 -0.00215 0.00474

D9 3.13954 0.00001 0.00081 0.00000 0.00081 3.14036

D10 -1.07147 0.00000 0.00076 0.00009 0.00085 -1.07062

D11 1.03808 -0.00001 0.00075 0.00006 0.00081 1.03889

D12 1.04415 0.00002 0.00038 -0.00100 -0.00062 1.04353

D13 3.11632 0.00001 0.00033 -0.00091 -0.00058 3.11573

D14 -1.05732 0.00001 0.00031 -0.00094 -0.00062 -1.05794

D15 -0.99462 0.00000 0.00061 0.00030 0.00092 -0.99371

D16 1.07754 0.00000 0.00056 0.00039 0.00095 1.07850

D17 -3.09609 -0.00001 0.00055 0.00036 0.00091 -3.09518

D18 -3.08832 -0.00001 -0.00088 -0.00676 -0.00763 -3.09595

D19 -0.88111 0.00002 -0.00093 -0.00603 -0.00696 -0.88807

D20 1.22319 0.00000 -0.00106 -0.00650 -0.00756 1.21562

D21 1.82163 -0.00004 -0.00069 -0.00151 -0.00221 1.81942

D22 -1.14033 0.00002 -0.00017 -0.00279 -0.00296 -1.14328

D23 2.59565 0.00004 0.00101 0.00335 0.00435 2.60000

D24 -0.72704 -0.00002 0.00047 0.00465 0.00512 -0.72192

D25 -3.03559 0.00001 -0.00058 -0.00826 -0.00884 -3.04443

D26 -0.91567 -0.00002 -0.00042 -0.00949 -0.00990 -0.92557

D27 1.12155 0.00000 -0.00033 -0.00884 -0.00917 1.11238

D28 -3.12397 0.00000 0.00051 -0.00370 -0.00319 -3.12716

D29 -1.00371 0.00000 0.00052 -0.00343 -0.00291 -1.00662

D30 1.03608 -0.00001 0.00048 -0.00395 -0.00346 1.03262

D31 1.07502 0.00001 0.00026 -0.00221 -0.00195 1.07307

D32 -3.08790 0.00001 0.00026 -0.00193 -0.00167 -3.08957

D33 -1.04811 0.00000 0.00023 -0.00245 -0.00222 -1.05034

D34 -1.02558 -0.00001 0.00027 -0.00257 -0.00230 -1.02788

D35 1.09468 -0.00001 0.00027 -0.00229 -0.00202 1.09266

D36 3.13447 -0.00002 0.00023 -0.00281 -0.00258 3.13189

D37 -3.13304 0.00000 -0.00023 0.00371 0.00348 -3.12956

D38 -1.00307 -0.00001 -0.00014 0.00233 0.00219 -1.00087

D39 1.01940 0.00000 -0.00016 0.00267 0.00250 1.02190

D40 1.02465 0.00000 -0.00015 0.00302 0.00286 1.02751

D41 -3.12856 -0.00001 -0.00006 0.00163 0.00157 -3.12699

D42 -1.10610 0.00000 -0.00009 0.00197 0.00188 -1.10422

D43 -1.00481 0.00000 -0.00018 0.00329 0.00311 -1.00170

D44 1.12517 -0.00001 -0.00009 0.00191 0.00182 1.12699

D45 -3.13556 0.00000 -0.00011 0.00224 0.00213 -3.13343

D46 3.13799 -0.00001 0.00052 -0.00149 -0.00098 3.13701

D47 -1.05005 0.00000 0.00046 -0.00094 -0.00048 -1.05054

D48 1.04205 -0.00001 0.00053 -0.00095 -0.00042 1.04163

D49 1.01174 0.00000 0.00045 -0.00036 0.00010 1.01183

D50 3.10688 0.00001 0.00039 0.00019 0.00059 3.10747

D51 -1.08420 0.00000 0.00046 0.00019 0.00065 -1.08355

D52 -1.01734 0.00000 0.00047 -0.00049 -0.00002 -1.01736

D53 1.07780 0.00000 0.00041 0.00006 0.00048 1.07828

D54 -3.11328 0.00000 0.00048 0.00006 0.00054 -3.11274

Item Value Threshold Converged?

Maximum Force 0.000143 0.000450 YES

RMS Force 0.000025 0.000300 YES

Maximum Displacement 0.057584 0.001800 NO

RMS Displacement 0.011706 0.001200 NO

Predicted change in Energy=-6.022045D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:59:15 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.100439 -0.398896 -0.189801

2 6 0 -2.840557 0.071352 0.476126

3 8 0 -4.911826 0.326014 -0.722070

4 8 0 -4.236816 -1.743285 -0.182798

5 6 0 -2.288915 -0.824006 1.568202

6 16 0 -1.585056 0.295679 -0.945966

7 6 0 -0.119204 0.768240 -0.105907

8 16 0 1.080623 -0.560001 0.001763

9 16 0 0.023844 2.250150 0.758492

10 6 0 2.685058 0.335177 -0.015695

11 6 0 3.843556 -0.654561 -0.068397

12 6 0 5.201501 0.053491 -0.063873

13 6 0 6.373563 -0.923586 -0.133315

14 1 0 -3.026100 1.078127 0.847143

15 1 0 -5.055348 -1.953457 -0.662941

16 1 0 -1.377563 -0.385015 1.976201

17 1 0 -3.011604 -0.918824 2.384805

18 1 0 -2.056023 -1.821592 1.195354

19 1 0 2.688913 0.991816 -0.888491

20 1 0 2.742348 0.957829 0.877263

21 1 0 3.788734 -1.336362 0.788553

22 1 0 3.760673 -1.275734 -0.967436

23 1 0 5.250079 0.746090 -0.912267

24 1 0 5.287408 0.668230 0.839764

25 1 0 7.333383 -0.398502 -0.133651

26 1 0 6.371790 -1.607720 0.721453

27 1 0 6.330140 -1.532292 -1.042288

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.500631 0.000000

3 O 1.211262 2.406384 0.000000

4 O 1.351307 2.382568 2.242422 0.000000

5 C 2.559866 1.516116 3.667092 2.775860 0.000000

6 S 2.716867 1.910222 3.334434 3.430981 2.840802

7 C 4.149636 2.868828 4.852262 4.823733 3.169469

8 S 5.187104 3.999910 6.100689 5.450631 3.725213

9 S 4.992636 3.609942 5.500473 5.914962 3.931275

10 C 6.827309 5.553730 7.629660 7.229127 5.347228

11 C 7.949035 6.745429 8.834338 8.154190 6.349359

12 C 9.313785 8.060186 10.138386 9.608557 7.716216

13 C 10.487288 9.287698 11.369615 10.642110 8.828567

14 H 2.100251 1.088888 2.565943 3.238361 2.163673

15 H 1.884775 3.209771 2.284751 0.971959 3.729184

16 H 3.479341 2.144493 4.503027 3.831645 1.090752

17 H 2.843323 2.157027 3.848785 2.962004 1.094582

18 H 2.849974 2.171640 4.055162 2.580948 1.090152

19 H 6.965453 5.769269 7.631659 7.479605 5.840490

20 H 7.057128 5.667060 7.844963 7.558338 5.382001

21 H 8.004690 6.784302 8.985834 8.094353 6.148835

22 H 7.947996 6.890192 8.822587 8.049477 6.575031

23 H 9.448023 8.236583 10.172363 9.835156 8.090387

24 H 9.504232 8.157960 10.323798 9.877848 7.756163

25 H 11.433960 10.203021 12.280729 11.648191 9.780898

26 H 10.581079 9.367327 11.538765 10.647938 8.737220

27 H 10.526551 9.432864 11.399019 10.603951 9.033517

6 7 8 9 10

6 S 0.000000

7 C 1.754348 0.000000

8 S 2.955710 1.793154 0.000000

9 S 3.051835 1.721542 3.096186 0.000000

10 C 4.370451 2.838938 1.837352 3.368760 0.000000

11 C 5.580584 4.210610 2.765440 4.869424 1.524623

12 C 6.847927 5.368662 4.166811 5.684164 2.532617

13 C 8.092381 6.709624 5.307133 7.154499 3.899152

14 H 2.429830 3.074798 4.501478 3.268587 5.823555

15 H 4.145075 5.664225 6.327219 6.744552 8.097572

16 H 3.007567 2.692329 3.157801 3.223484 4.581617

17 H 3.821530 4.173225 4.749101 4.679876 6.307684

18 H 3.047934 3.485940 3.585362 4.593014 5.347537

19 H 4.330672 2.923687 2.405677 3.376173 1.092228

20 H 4.742261 3.031674 2.414879 3.012384 1.090115

21 H 5.877902 4.527845 2.925002 5.199842 2.158461

22 H 5.571949 4.469172 2.938416 5.419831 2.158192

23 H 6.850043 5.429541 4.463820 5.689215 2.748095

24 H 7.110442 5.489603 4.461820 5.496742 2.759521

25 H 8.982221 7.543415 6.256311 7.825639 4.707347

26 H 8.349528 6.961517 5.441702 7.428388 4.232048

27 H 8.124105 6.911099 5.439928 7.570934 4.222316

11 12 13 14 15

11 C 0.000000

12 C 1.531461 0.000000

13 C 2.545099 1.527492 0.000000

14 H 7.143710 8.341058 9.660322 0.000000

15 H 9.012830 10.468509 11.487435 3.948254 0.000000

16 H 5.613654 6.902048 8.051091 2.476537 4.790740

17 H 7.285687 8.625341 9.717114 2.520403 3.812626

18 H 6.145247 7.600871 8.580775 3.077446 3.530807

19 H 2.171708 2.805984 4.220866 5.973378 8.288491

20 H 2.169501 2.784062 4.212686 5.769781 8.464744

21 H 1.096457 2.157366 2.775170 7.230156 8.983620

22 H 1.095900 2.158529 2.765314 7.409025 8.847274

23 H 2.156908 1.096278 2.157962 8.467640 10.656057

24 H 2.158528 1.096287 2.158819 8.323610 10.775156

25 H 3.499817 2.180387 1.094060 10.510056 12.497148

26 H 2.815021 2.178517 1.094838 9.774964 11.515884

27 H 2.811045 2.178492 1.094824 9.895628 11.399589

16 17 18 19 20

16 H 0.000000

17 H 1.766918 0.000000

18 H 1.770250 1.772827 0.000000

19 H 5.161235 6.845502 5.896787 0.000000

20 H 4.470409 6.237184 5.554343 1.766890 0.000000

21 H 5.385739 6.997639 5.878956 3.072864 2.523114

22 H 5.988309 7.564961 6.229733 2.509319 3.070620

23 H 7.317670 9.049753 8.025845 2.573037 3.088037

24 H 6.842708 8.589499 7.762193 3.137475 2.561758

25 H 8.962825 10.659836 9.589181 4.906513 4.892769

26 H 7.944928 9.554549 8.443836 4.786763 4.447378

27 H 8.356805 9.969427 8.684381 4.433205 4.770496

21 22 23 24 25

21 H 0.000000

22 H 1.757259 0.000000

23 H 3.060216 2.511801 0.000000

24 H 2.503405 3.062007 1.754158 0.000000

25 H 3.780817 3.772133 2.501297 2.504290 0.000000

26 H 2.598138 3.127379 3.076962 2.523853 1.765806

27 H 3.138329 2.583328 2.524769 3.077614 1.765672

26 27

26 H 0.000000

27 H 1.765844 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 8.96D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.107156 -0.457669 -0.118546

2 6 0 -2.842674 0.110662 0.455891

3 8 0 -4.922467 0.174866 -0.752835

4 8 0 -4.243185 -1.783973 0.101552

5 6 0 -2.283083 -0.601581 1.671694

6 16 0 -1.597367 0.106554 -0.992605

7 6 0 -0.125681 0.704470 -0.248041

8 16 0 1.075172 -0.591208 0.059482

9 16 0 0.023185 2.304119 0.370558

10 6 0 2.679246 0.288537 -0.110389

11 6 0 3.837557 -0.698161 -0.014366

12 6 0 5.195344 0.000498 -0.131253

13 6 0 6.367098 -0.976353 -0.053855

14 1 0 -3.025795 1.163549 0.664630

15 1 0 -5.065065 -2.066561 -0.333605

16 1 0 -1.368949 -0.104514 1.998838

17 1 0 -2.999926 -0.565651 2.498105

18 1 0 -2.052630 -1.645726 1.459363

19 1 0 2.676750 0.799164 -1.075902

20 1 0 2.742748 1.044288 0.672657

21 1 0 3.788979 -1.236089 0.939831

22 1 0 3.748419 -1.453388 -0.803469

23 1 0 5.237737 0.550445 -1.078663

24 1 0 5.287540 0.750095 0.663384

25 1 0 7.326775 -0.458774 -0.143848

26 1 0 6.371553 -1.516978 0.898183

27 1 0 6.317345 -1.720873 -0.855012

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3095258 0.1934376 0.1808008

Leave Link 202 at Sat Aug 17 17:59:15 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.4109758816 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0550111090 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.3559647726 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

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Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2323

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.94D-10

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 101

GePol: Fraction of low-weight points (<1% of avg) = 4.35%

GePol: Cavity surface area = 309.358 Ang\*\*2

GePol: Cavity volume = 320.476 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057968165 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.3501679562 Hartrees.

Leave Link 301 at Sat Aug 17 17:59:15 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:59:16 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:59:16 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999996 -0.002971 -0.000176 0.000007 Ang= -0.34 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.63026709094

Leave Link 401 at Sat Aug 17 17:59:16 2019, MaxMem= 1342177280 cpu: 7.7

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16188987.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.33D-15 for 2322.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.63D-15 for 2311 1784.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.11D-15 for 2322.

Iteration 1 A^-1\*A deviation from orthogonality is 4.82D-12 for 802 798.

E= -1658.67653653388

DIIS: error= 1.07D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67653653388 IErMin= 1 ErrMin= 1.07D-03

ErrMax= 1.07D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.21D-03 BMatP= 1.21D-03

IDIUse=3 WtCom= 9.89D-01 WtEn= 1.07D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.428 Goal= None Shift= 0.000

Gap= 0.484 Goal= None Shift= 0.000

GapD= 0.428 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=6.91D-05 MaxDP=2.30D-03 OVMax= 5.77D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 6.91D-05 CP: 1.00D+00

E= -1658.67702906681 Delta-E= -0.000492532924 Rises=F Damp=F

DIIS: error= 1.53D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67702906681 IErMin= 2 ErrMin= 1.53D-04

ErrMax= 1.53D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.07D-05 BMatP= 1.21D-03

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.53D-03

Coeff-Com: -0.693D-01 0.107D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.692D-01 0.107D+01

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.04D-05 MaxDP=3.53D-04 DE=-4.93D-04 OVMax= 8.12D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 9.37D-06 CP: 1.00D+00 1.07D+00

E= -1658.67703326172 Delta-E= -0.000004194917 Rises=F Damp=F

DIIS: error= 1.41D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67703326172 IErMin= 3 ErrMin= 1.41D-04

ErrMax= 1.41D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.19D-05 BMatP= 2.07D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.41D-03

Coeff-Com: -0.360D-01 0.491D+00 0.545D+00

Coeff-En: 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.359D-01 0.491D+00 0.545D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=7.04D-06 MaxDP=3.68D-04 DE=-4.19D-06 OVMax= 6.48D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 4.91D-06 CP: 1.00D+00 1.08D+00 4.73D-01

E= -1658.67703456336 Delta-E= -0.000001301638 Rises=F Damp=F

DIIS: error= 9.92D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67703456336 IErMin= 4 ErrMin= 9.92D-05

ErrMax= 9.92D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.53D-06 BMatP= 1.19D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.110D-01 0.145D+00 0.393D+00 0.472D+00

Coeff: -0.110D-01 0.145D+00 0.393D+00 0.472D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.95D-06 MaxDP=1.32D-04 DE=-1.30D-06 OVMax= 2.83D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.13D-06 CP: 1.00D+00 1.08D+00 6.64D-01 5.84D-01

E= -1658.67703561990 Delta-E= -0.000001056540 Rises=F Damp=F

DIIS: error= 7.25D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67703561990 IErMin= 5 ErrMin= 7.25D-06

ErrMax= 7.25D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.50D-08 BMatP= 5.53D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.263D-02 0.299D-01 0.138D+00 0.200D+00 0.634D+00

Coeff: -0.263D-02 0.299D-01 0.138D+00 0.200D+00 0.634D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.28D-07 MaxDP=3.17D-05 DE=-1.06D-06 OVMax= 3.76D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 4.07D-07 CP: 1.00D+00 1.08D+00 6.86D-01 6.09D-01 7.87D-01

E= -1658.67703563513 Delta-E= -0.000000015231 Rises=F Damp=F

DIIS: error= 4.14D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67703563513 IErMin= 6 ErrMin= 4.14D-06

ErrMax= 4.14D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.96D-08 BMatP= 8.50D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.638D-03-0.128D-01 0.524D-02 0.270D-01 0.353D+00 0.627D+00

Coeff: 0.638D-03-0.128D-01 0.524D-02 0.270D-01 0.353D+00 0.627D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.17D-07 MaxDP=9.18D-06 DE=-1.52D-08 OVMax= 2.23D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.44D-07 CP: 1.00D+00 1.08D+00 6.88D-01 6.27D-01 8.66D-01

CP: 7.55D-01

E= -1658.67703563902 Delta-E= -0.000000003890 Rises=F Damp=F

DIIS: error= 9.12D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67703563902 IErMin= 7 ErrMin= 9.12D-07

ErrMax= 9.12D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.30D-09 BMatP= 1.96D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.458D-03-0.806D-02-0.429D-02 0.333D-02 0.143D+00 0.314D+00

Coeff-Com: 0.551D+00

Coeff: 0.458D-03-0.806D-02-0.429D-02 0.333D-02 0.143D+00 0.314D+00

Coeff: 0.551D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=9.26D-08 MaxDP=3.40D-06 DE=-3.89D-09 OVMax= 1.05D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 7.44D-08 CP: 1.00D+00 1.08D+00 6.89D-01 6.25D-01 8.98D-01

CP: 8.07D-01 7.88D-01

E= -1658.67703563932 Delta-E= -0.000000000292 Rises=F Damp=F

DIIS: error= 3.63D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67703563932 IErMin= 8 ErrMin= 3.63D-07

ErrMax= 3.63D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.60D-10 BMatP= 1.30D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.119D-03-0.178D-02-0.312D-02-0.319D-02 0.978D-02 0.490D-01

Coeff-Com: 0.311D+00 0.638D+00

Coeff: 0.119D-03-0.178D-02-0.312D-02-0.319D-02 0.978D-02 0.490D-01

Coeff: 0.311D+00 0.638D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.17D-08 MaxDP=1.86D-06 DE=-2.92D-10 OVMax= 4.77D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.65D-08 CP: 1.00D+00 1.08D+00 6.90D-01 6.28D-01 9.02D-01

CP: 8.38D-01 9.51D-01 8.35D-01

E= -1658.67703563938 Delta-E= -0.000000000064 Rises=F Damp=F

DIIS: error= 2.05D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67703563938 IErMin= 9 ErrMin= 2.05D-07

ErrMax= 2.05D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.96D-11 BMatP= 2.60D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.147D-04 0.491D-03-0.111D-02-0.265D-02-0.220D-01-0.302D-01

Coeff-Com: 0.927D-01 0.404D+00 0.559D+00

Coeff: -0.147D-04 0.491D-03-0.111D-02-0.265D-02-0.220D-01-0.302D-01

Coeff: 0.927D-01 0.404D+00 0.559D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.02D-08 MaxDP=1.03D-06 DE=-6.37D-11 OVMax= 2.82D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 9.77D-09 CP: 1.00D+00 1.08D+00 6.90D-01 6.27D-01 9.05D-01

CP: 8.53D-01 1.00D+00 9.99D-01 8.30D-01

E= -1658.67703563938 Delta-E= -0.000000000001 Rises=F Damp=F

DIIS: error= 5.87D-08 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1658.67703563938 IErMin=10 ErrMin= 5.87D-08

ErrMax= 5.87D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.36D-12 BMatP= 6.96D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.290D-04 0.566D-03 0.760D-04-0.607D-03-0.117D-01-0.226D-01

Coeff-Com: -0.197D-01 0.563D-01 0.230D+00 0.768D+00

Coeff: -0.290D-04 0.566D-03 0.760D-04-0.607D-03-0.117D-01-0.226D-01

Coeff: -0.197D-01 0.563D-01 0.230D+00 0.768D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=9.12D-09 MaxDP=3.46D-07 DE=-9.09D-13 OVMax= 1.61D-06

Error on total polarization charges = 0.04161

SCF Done: E(UB3LYP) = -1658.67703564 A.U. after 10 cycles

NFock= 10 Conv=0.91D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655238963185D+03 PE=-6.147467397217D+03 EE= 1.731201230436D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.64

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 17:59:39 2019, MaxMem= 1342177280 cpu: 257.3

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 335

Leave Link 701 at Sat Aug 17 17:59:40 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:59:40 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 17:59:43 2019, MaxMem= 1342177280 cpu: 38.2

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.41849119D+00-2.95957810D+00 6.17813992D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000207617 -0.000225595 0.000237433

2 6 -0.000008418 0.000090468 -0.000131365

3 8 -0.000156872 0.000148253 -0.000082251

4 8 -0.000028936 0.000075587 -0.000020009

5 6 -0.000010077 -0.000114181 0.000020729

6 16 0.000109010 -0.000000043 -0.000047089

7 6 0.000061906 -0.000048203 -0.000090296

8 16 -0.000011894 0.000165733 0.000125096

9 16 -0.000057936 0.000064222 0.000138976

10 6 0.000053216 -0.000095784 0.000039438

11 6 0.000022202 -0.000014896 -0.000007003

12 6 0.000045343 -0.000091258 -0.000136233

13 6 -0.000060012 0.000125071 -0.000043559

14 1 -0.000075861 0.000029251 0.000121363

15 1 -0.000037755 -0.000007109 -0.000077548

16 1 0.000010699 -0.000021761 -0.000009027

17 1 -0.000061684 -0.000072232 0.000042044

18 1 0.000019153 -0.000020328 -0.000006098

19 1 0.000047654 0.000141552 -0.000032960

20 1 -0.000135392 -0.000062317 0.000066553

21 1 -0.000050228 -0.000039000 0.000008082

22 1 0.000085480 -0.000036595 -0.000118660

23 1 0.000003259 0.000106649 -0.000041405

24 1 -0.000000483 -0.000045340 0.000071636

25 1 0.000043247 0.000050701 0.000005109

26 1 -0.000003913 -0.000083385 0.000026167

27 1 -0.000009326 -0.000019458 -0.000059123

-------------------------------------------------------------------

Cartesian Forces: Max 0.000237433 RMS 0.000083664

Leave Link 716 at Sat Aug 17 17:59:43 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000438436 RMS 0.000074663

Search for a local minimum.

Step number 64 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .74663D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43 45 44 47 46

49 48 51 50 53

54 55 56 52 57

59 60 61 62 63

64

DE= -1.38D-05 DEPred=-6.02D-07 R= 2.30D+01

TightC=F SS= 1.41D+00 RLast= 4.29D-02 DXNew= 1.4232D-01 1.2858D-01

Trust test= 2.30D+01 RLast= 4.29D-02 DXMaxT set to 1.29D-01

ITU= 1 1 1 -1 1 0 -1 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 1 1 1 1 1 -1 -1 0 -1 -1 -1 0 -1 0 0 -1 -1 0 0 -1

ITU= 0 0 -1 1 -1 1 -1 1 1 -1 1 -1 1 1 -1 0 0 -1 0 0

ITU= -1 -1 0 0

Eigenvalues --- 0.00034 0.00154 0.00231 0.00282 0.00331

Eigenvalues --- 0.00342 0.00604 0.00790 0.01731 0.01929

Eigenvalues --- 0.03369 0.03559 0.03601 0.03911 0.04407

Eigenvalues --- 0.04765 0.04805 0.04818 0.05112 0.05379

Eigenvalues --- 0.05468 0.05537 0.05602 0.05747 0.07892

Eigenvalues --- 0.08217 0.08316 0.10761 0.11047 0.11739

Eigenvalues --- 0.12166 0.14070 0.14929 0.15241 0.15538

Eigenvalues --- 0.15855 0.16059 0.16383 0.17037 0.17485

Eigenvalues --- 0.18525 0.18856 0.20405 0.21634 0.22353

Eigenvalues --- 0.22756 0.23285 0.24705 0.25579 0.26720

Eigenvalues --- 0.27838 0.28055 0.28934 0.29292 0.29882

Eigenvalues --- 0.30860 0.31477 0.33575 0.33731 0.33869

Eigenvalues --- 0.33941 0.33967 0.34009 0.34081 0.34108

Eigenvalues --- 0.34175 0.34252 0.34526 0.35010 0.35567

Eigenvalues --- 0.35852 0.37346 0.49359 0.53435 0.86521

En-DIIS/RFO-DIIS IScMMF= 0 using points: 64 63 62 61 60

RFO step: Lambda=-1.73109923D-06.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= -4.63D-05 SmlDif= 1.00D-05

RMS Error= 0.2332920078D-03 NUsed= 5 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.14355 0.61001 0.15964 0.04980 0.03700

Iteration 1 RMS(Cart)= 0.00980192 RMS(Int)= 0.00002483

Iteration 2 RMS(Cart)= 0.00004375 RMS(Int)= 0.00000020

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000020

ITry= 1 IFail=0 DXMaxC= 3.13D-02 DCOld= 1.00D+10 DXMaxT= 1.29D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83578 0.00000 -0.00026 0.00004 -0.00022 2.83556

R2 2.28895 0.00023 0.00018 0.00033 0.00052 2.28947

R3 2.55360 -0.00003 -0.00031 0.00012 -0.00019 2.55341

R4 2.86504 0.00009 0.00009 0.00040 0.00049 2.86553

R5 3.60980 0.00018 0.00058 0.00062 0.00120 3.61100

R6 2.05770 0.00008 0.00019 0.00007 0.00026 2.05796

R7 1.83674 0.00006 0.00012 0.00006 0.00018 1.83692

R8 2.06122 0.00001 -0.00001 0.00016 0.00015 2.06137

R9 2.06846 0.00008 0.00020 0.00016 0.00036 2.06882

R10 2.06009 -0.00001 -0.00006 0.00009 0.00003 2.06012

R11 3.31524 0.00002 0.00014 0.00009 0.00023 3.31547

R12 3.38857 0.00001 -0.00043 0.00005 -0.00038 3.38819

R13 3.25324 0.00010 0.00055 0.00021 0.00076 3.25400

R14 3.47209 -0.00003 -0.00017 -0.00009 -0.00026 3.47183

R15 2.88112 0.00014 0.00028 0.00021 0.00049 2.88161

R16 2.06401 0.00012 0.00023 0.00021 0.00044 2.06445

R17 2.06002 0.00000 0.00002 0.00018 0.00020 2.06022

R18 2.89404 0.00002 0.00009 0.00008 0.00016 2.89421

R19 2.07200 0.00005 0.00015 0.00009 0.00024 2.07225

R20 2.07095 0.00010 0.00017 0.00015 0.00032 2.07128

R21 2.88654 -0.00005 -0.00035 0.00002 -0.00033 2.88621

R22 2.07167 0.00010 0.00025 0.00014 0.00039 2.07205

R23 2.07168 0.00003 0.00008 0.00010 0.00018 2.07186

R24 2.06747 0.00006 0.00014 0.00012 0.00026 2.06773

R25 2.06894 0.00010 0.00028 0.00016 0.00043 2.06938

R26 2.06892 0.00004 0.00009 0.00012 0.00021 2.06912

A1 2.17714 -0.00003 -0.00060 0.00016 -0.00044 2.17670

A2 1.97599 0.00010 0.00095 -0.00037 0.00058 1.97657

A3 2.12950 -0.00007 -0.00037 0.00021 -0.00016 2.12934

A4 2.02647 -0.00008 0.00004 -0.00100 -0.00096 2.02551

A5 1.83200 0.00001 -0.00111 0.00016 -0.00095 1.83104

A6 1.87327 0.00002 0.00001 -0.00051 -0.00050 1.87276

A7 1.94599 0.00007 0.00047 0.00065 0.00112 1.94711

A8 1.94185 -0.00002 -0.00017 0.00029 0.00013 1.94197

A9 1.83079 0.00002 0.00079 0.00052 0.00131 1.83210

A10 1.87293 0.00003 -0.00036 0.00031 -0.00006 1.87287

A11 1.91321 -0.00004 -0.00033 0.00051 0.00018 1.91339

A12 1.92656 -0.00001 -0.00012 -0.00046 -0.00059 1.92597

A13 1.95173 0.00005 0.00050 0.00013 0.00063 1.95236

A14 1.88331 0.00002 0.00010 -0.00007 0.00003 1.88334

A15 1.89413 -0.00001 0.00002 0.00007 0.00010 1.89423

A16 1.89329 -0.00001 -0.00018 -0.00018 -0.00036 1.89293

A17 1.79704 0.00022 0.00130 0.00071 0.00200 1.79905

A18 1.96959 -0.00020 -0.00027 -0.00020 -0.00047 1.96912

A19 2.14329 0.00001 0.00005 0.00022 0.00026 2.14355

A20 2.15541 0.00018 0.00010 -0.00018 -0.00008 2.15533

A21 1.79551 0.00044 0.00058 0.00024 0.00083 1.79634

A22 1.92578 0.00003 0.00048 -0.00019 0.00030 1.92608

A23 1.87925 0.00007 0.00044 0.00060 0.00104 1.88028

A24 1.89272 -0.00015 -0.00093 -0.00031 -0.00124 1.89148

A25 1.93903 -0.00006 0.00033 0.00007 0.00041 1.93944

A26 1.93818 0.00011 -0.00006 -0.00010 -0.00016 1.93802

A27 1.88704 -0.00001 -0.00029 -0.00006 -0.00035 1.88669

A28 1.95361 -0.00004 -0.00059 0.00002 -0.00056 1.95304

A29 1.91629 -0.00004 -0.00039 -0.00038 -0.00077 1.91552

A30 1.91649 0.00009 0.00073 0.00030 0.00104 1.91753

A31 1.90659 0.00006 0.00027 0.00002 0.00029 1.90688

A32 1.90874 -0.00006 -0.00023 -0.00011 -0.00034 1.90840

A33 1.85973 0.00000 0.00024 0.00015 0.00039 1.86011

A34 1.96546 0.00005 0.00054 -0.00002 0.00052 1.96599

A35 1.90614 0.00000 0.00013 0.00002 0.00014 1.90629

A36 1.90834 -0.00004 -0.00054 -0.00008 -0.00062 1.90772

A37 1.91233 0.00001 0.00054 0.00011 0.00065 1.91299

A38 1.91350 -0.00004 -0.00071 -0.00008 -0.00079 1.91271

A39 1.85475 0.00002 0.00001 0.00006 0.00007 1.85483

A40 1.94569 -0.00003 -0.00026 -0.00005 -0.00031 1.94538

A41 1.94225 0.00000 -0.00011 -0.00003 -0.00014 1.94211

A42 1.94223 0.00002 0.00062 -0.00005 0.00057 1.94280

A43 1.87713 0.00001 -0.00019 0.00002 -0.00017 1.87696

A44 1.87694 0.00002 0.00023 0.00005 0.00028 1.87722

A45 1.87623 -0.00002 -0.00030 0.00006 -0.00024 1.87599

D1 2.68690 -0.00003 0.01148 -0.01192 -0.00044 2.68646

D2 -1.43902 0.00001 0.01126 -0.01161 -0.00035 -1.43936

D3 0.50238 0.00004 0.01166 -0.01117 0.00050 0.50287

D4 -0.49033 -0.00004 0.01108 -0.01199 -0.00091 -0.49124

D5 1.66693 0.00000 0.01086 -0.01168 -0.00081 1.66612

D6 -2.67486 0.00003 0.01127 -0.01123 0.00003 -2.67483

D7 -3.10232 0.00002 0.00240 0.00059 0.00298 -3.09933

D8 0.00474 0.00001 0.00201 0.00052 0.00253 0.00726

D9 3.14036 0.00003 0.00014 -0.00025 -0.00010 3.14026

D10 -1.07062 0.00002 -0.00001 -0.00030 -0.00031 -1.07094

D11 1.03889 0.00003 0.00001 -0.00077 -0.00075 1.03813

D12 1.04353 0.00002 0.00123 -0.00024 0.00099 1.04452

D13 3.11573 0.00002 0.00108 -0.00029 0.00078 3.11652

D14 -1.05794 0.00002 0.00110 -0.00076 0.00034 -1.05760

D15 -0.99371 -0.00003 0.00005 -0.00148 -0.00143 -0.99514

D16 1.07850 -0.00003 -0.00010 -0.00154 -0.00164 1.07686

D17 -3.09518 -0.00003 -0.00008 -0.00200 -0.00208 -3.09726

D18 -3.09595 0.00008 0.00698 0.00130 0.00828 -3.08767

D19 -0.88807 0.00003 0.00656 0.00058 0.00713 -0.88093

D20 1.21562 0.00004 0.00710 0.00160 0.00870 1.22432

D21 1.81942 0.00004 0.00107 -0.00021 0.00086 1.82028

D22 -1.14328 0.00008 0.00182 0.00078 0.00261 -1.14067

D23 2.60000 0.00000 -0.00372 0.00142 -0.00230 2.59770

D24 -0.72192 -0.00007 -0.00448 0.00046 -0.00402 -0.72594

D25 -3.04443 0.00010 0.00777 -0.00211 0.00566 -3.03877

D26 -0.92557 0.00008 0.00875 -0.00176 0.00699 -0.91858

D27 1.11238 0.00003 0.00815 -0.00167 0.00648 1.11885

D28 -3.12716 0.00004 0.00344 0.00042 0.00387 -3.12329

D29 -1.00662 0.00006 0.00312 0.00020 0.00332 -1.00329

D30 1.03262 0.00008 0.00361 0.00034 0.00395 1.03657

D31 1.07307 -0.00003 0.00236 -0.00025 0.00211 1.07519

D32 -3.08957 -0.00001 0.00205 -0.00047 0.00157 -3.08800

D33 -1.05034 0.00001 0.00253 -0.00034 0.00220 -1.04814

D34 -1.02788 -0.00005 0.00255 -0.00015 0.00240 -1.02549

D35 1.09266 -0.00004 0.00223 -0.00037 0.00186 1.09452

D36 3.13189 -0.00001 0.00272 -0.00024 0.00248 3.13437

D37 -3.12956 -0.00006 -0.00255 -0.00049 -0.00304 -3.13260

D38 -1.00087 -0.00002 -0.00141 -0.00035 -0.00176 -1.00263

D39 1.02190 -0.00002 -0.00163 -0.00031 -0.00194 1.01996

D40 1.02751 -0.00002 -0.00186 -0.00004 -0.00190 1.02561

D41 -3.12699 0.00002 -0.00072 0.00010 -0.00062 -3.12761

D42 -1.10422 0.00002 -0.00094 0.00014 -0.00080 -1.10501

D43 -1.00170 -0.00001 -0.00217 -0.00016 -0.00233 -1.00403

D44 1.12699 0.00003 -0.00103 -0.00002 -0.00105 1.12594

D45 -3.13343 0.00003 -0.00125 0.00002 -0.00123 -3.13466

D46 3.13701 0.00003 0.00141 0.00040 0.00181 3.13882

D47 -1.05054 0.00002 0.00091 0.00038 0.00129 -1.04925

D48 1.04163 0.00002 0.00087 0.00040 0.00127 1.04290

D49 1.01183 0.00000 0.00050 0.00031 0.00081 1.01264

D50 3.10747 -0.00001 0.00000 0.00029 0.00029 3.10776

D51 -1.08355 -0.00002 -0.00004 0.00031 0.00027 -1.08328

D52 -1.01736 0.00000 0.00058 0.00022 0.00080 -1.01656

D53 1.07828 -0.00001 0.00008 0.00020 0.00028 1.07856

D54 -3.11274 -0.00002 0.00004 0.00022 0.00026 -3.11248

Item Value Threshold Converged?

Maximum Force 0.000438 0.000450 YES

RMS Force 0.000075 0.000300 YES

Maximum Displacement 0.031336 0.001800 NO

RMS Displacement 0.009807 0.001200 NO

Predicted change in Energy=-3.379100D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:59:43 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.097630 -0.406029 -0.194812

2 6 0 -2.844101 0.074587 0.475422

3 8 0 -4.910573 0.312308 -0.734194

4 8 0 -4.226296 -1.751050 -0.183750

5 6 0 -2.293919 -0.813640 1.574395

6 16 0 -1.583441 0.299531 -0.942856

7 6 0 -0.118382 0.771215 -0.100668

8 16 0 1.080511 -0.557618 0.006740

9 16 0 0.023476 2.251434 0.767618

10 6 0 2.686141 0.335107 -0.012177

11 6 0 3.843409 -0.655980 -0.073309

12 6 0 5.202021 0.050942 -0.064701

13 6 0 6.373678 -0.926052 -0.138153

14 1 0 -3.038307 1.081659 0.841571

15 1 0 -5.039868 -1.967740 -0.669589

16 1 0 -1.387050 -0.368432 1.985849

17 1 0 -3.021131 -0.908337 2.387239

18 1 0 -2.054225 -1.811909 1.207690

19 1 0 2.688516 0.997177 -0.881157

20 1 0 2.746589 0.952621 0.884262

21 1 0 3.788022 -1.343409 0.779260

22 1 0 3.759840 -1.270916 -0.976770

23 1 0 5.251276 0.748665 -0.909113

24 1 0 5.287806 0.660266 0.842725

25 1 0 7.333662 -0.401002 -0.133599

26 1 0 6.370347 -1.615175 0.712888

27 1 0 6.331789 -1.529860 -1.050589

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.500513 0.000000

3 O 1.211535 2.406239 0.000000

4 O 1.351206 2.382839 2.242470 0.000000

5 C 2.559221 1.516374 3.666636 2.775589 0.000000

6 S 2.716344 1.910857 3.333693 3.430132 2.842618

7 C 4.150805 2.871710 4.855619 4.821170 3.170262

8 S 5.184279 4.002740 6.099085 5.442681 3.729593

9 S 4.997189 3.612069 5.510035 5.914858 3.926307

10 C 6.826579 5.557805 7.630982 7.222415 5.351432

11 C 7.945901 6.749639 8.832132 8.144416 6.356617

12 C 9.311780 8.064265 10.138100 9.599714 7.721609

13 C 10.484366 9.292213 11.367635 10.632129 8.835876

14 H 2.099875 1.089025 2.565213 3.238340 2.164095

15 H 1.884719 3.209913 2.284625 0.972056 3.729295

16 H 3.479072 2.144914 4.503027 3.831463 1.090833

17 H 2.842209 2.156971 3.847506 2.961853 1.094770

18 H 2.849388 2.172324 4.054865 2.580253 1.090168

19 H 6.963607 5.770730 7.631303 7.473537 5.842384

20 H 7.060713 5.673968 7.852485 7.554576 5.385414

21 H 8.000687 6.788821 8.983178 8.082255 6.156533

22 H 7.943508 6.894294 8.817114 8.039763 6.585252

23 H 9.446988 8.240537 10.172717 9.828484 8.095590

24 H 9.502624 8.161241 10.325438 9.868446 7.758240

25 H 11.431457 10.207054 12.279691 11.638633 9.786614

26 H 10.576601 9.371113 11.535527 10.635378 8.743807

27 H 10.524644 9.439276 11.396683 10.595919 9.044686

6 7 8 9 10

6 S 0.000000

7 C 1.754470 0.000000

8 S 2.955179 1.792952 0.000000

9 S 3.052512 1.721945 3.096293 0.000000

10 C 4.369984 2.839607 1.837216 3.371969 0.000000

11 C 5.578514 4.211107 2.765807 4.873613 1.524880

12 C 6.846565 5.369057 4.166808 5.687903 2.532422

13 C 8.091066 6.710363 5.307952 7.158345 3.899272

14 H 2.431571 3.083853 4.510968 3.278468 5.835711

15 H 4.142714 5.660969 6.317033 6.745698 8.088665

16 H 3.010325 2.694785 3.168836 3.215178 4.591074

17 H 3.823013 4.175707 4.755339 4.677281 6.314768

18 H 3.050354 3.483076 3.583587 4.584894 5.344980

19 H 4.328988 2.922139 2.406538 3.375508 1.092460

20 H 4.744897 3.034972 2.413852 3.019249 1.090220

21 H 5.875164 4.528344 2.923161 5.205270 2.158224

22 H 5.569391 4.469727 2.941920 5.423122 2.159301

23 H 6.849542 5.430223 4.465472 5.692068 2.748717

24 H 7.108619 5.489005 4.459085 5.500057 2.757761

25 H 8.981112 7.543748 6.256686 7.828565 4.707022

26 H 8.346876 6.961346 5.440537 7.432122 4.231158

27 H 8.124601 6.913899 5.444182 7.576204 4.224589

11 12 13 14 15

11 C 0.000000

12 C 1.531548 0.000000

13 C 2.545468 1.527316 0.000000

14 H 7.156424 8.353844 9.673481 0.000000

15 H 8.999382 10.456445 11.473298 3.948251 0.000000

16 H 5.628545 6.913500 8.065434 2.477657 4.790847

17 H 7.296567 8.634376 9.728328 2.519815 3.813375

18 H 6.144852 7.598835 8.580535 3.078181 3.530230

19 H 2.172401 2.807075 4.222711 5.980922 8.280302

20 H 2.169689 2.782571 4.210763 5.786492 8.460016

21 H 1.096586 2.157749 2.775150 7.244557 8.967753

22 H 1.096072 2.158486 2.766651 7.419958 8.832598

23 H 2.157240 1.096482 2.158435 8.478972 10.646308

24 H 2.158217 1.096384 2.158158 8.336769 10.763566

25 H 3.500073 2.180113 1.094196 10.522689 12.483837

26 H 2.814885 2.178435 1.095068 9.788373 11.499067

27 H 2.812610 2.178827 1.094933 9.909541 11.386460

16 17 18 19 20

16 H 0.000000

17 H 1.767154 0.000000

18 H 1.770389 1.772762 0.000000

19 H 5.166706 6.849340 5.894729 0.000000

20 H 4.477237 6.244093 5.549328 1.766935 0.000000

21 H 5.402574 7.009953 5.876639 3.073149 2.523363

22 H 6.006835 7.578231 6.234412 2.510204 3.071520

23 H 7.327761 9.057831 8.025443 2.574933 3.087272

24 H 6.849719 8.595608 7.755660 3.137130 2.558316

25 H 8.974627 10.669290 9.587603 4.908272 4.889742

26 H 7.959398 9.565717 8.441383 4.787614 4.444611

27 H 8.375521 9.984091 8.689338 4.437124 4.770746

21 22 23 24 25

21 H 0.000000

22 H 1.757752 0.000000

23 H 3.060799 2.511506 0.000000

24 H 2.503616 3.061814 1.754447 0.000000

25 H 3.780609 3.773578 2.501897 2.503003 0.000000

26 H 2.597435 3.128611 3.077490 2.523170 1.765993

27 H 3.139087 2.586005 2.525707 3.077530 1.766052

26 27

26 H 0.000000

27 H 1.765961 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 9.21D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.105143 -0.465460 -0.120677

2 6 0 -2.846870 0.117274 0.452654

3 8 0 -4.921922 0.155456 -0.765001

4 8 0 -4.233714 -1.790240 0.112101

5 6 0 -2.288850 -0.578991 1.678713

6 16 0 -1.596364 0.104708 -0.992148

7 6 0 -0.125338 0.706632 -0.249226

8 16 0 1.074306 -0.587895 0.066580

9 16 0 0.022697 2.309214 0.363073

10 6 0 2.679750 0.287728 -0.110039

11 6 0 3.836563 -0.701281 -0.015671

12 6 0 5.195194 -0.004128 -0.132879

13 6 0 6.366308 -0.981276 -0.053079

14 1 0 -3.038468 1.171039 0.649745

15 1 0 -5.050729 -2.082852 -0.325799

16 1 0 -1.379073 -0.073293 2.005043

17 1 0 -3.010243 -0.538025 2.501170

18 1 0 -2.051768 -1.624216 1.479308

19 1 0 2.675917 0.798048 -1.075973

20 1 0 2.746587 1.044045 0.672327

21 1 0 3.787268 -1.239250 0.938614

22 1 0 3.746556 -1.456182 -0.805225

23 1 0 5.238415 0.545341 -1.080765

24 1 0 5.287446 0.745886 0.661493

25 1 0 7.326294 -0.463728 -0.141600

26 1 0 6.369057 -1.521228 0.899611

27 1 0 6.317915 -1.726723 -0.853607

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3049136 0.1934998 0.1808311

Leave Link 202 at Sat Aug 17 17:59:43 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.2782404856 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0549919090 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.2232485765 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

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Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2323

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.89D-08

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 93

GePol: Fraction of low-weight points (<1% of avg) = 4.00%

GePol: Cavity surface area = 309.333 Ang\*\*2

GePol: Cavity volume = 320.465 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057886409 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.2174599356 Hartrees.

Leave Link 301 at Sat Aug 17 17:59:43 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 17:59:43 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:59:43 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999996 0.002846 0.000099 -0.000095 Ang= 0.33 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Generating alternative initial guess.

ExpMin= 7.71D-02 ExpMax= 9.34D+04 ExpMxC= 3.17D+03 IAcc=2 IRadAn= 4 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 4 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1658.63006054777

Leave Link 401 at Sat Aug 17 17:59:44 2019, MaxMem= 1342177280 cpu: 7.6

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16188987.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.33D-15 for 2310.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.97D-15 for 707 444.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.77D-15 for 2310.

Iteration 1 A^-1\*A deviation from orthogonality is 2.20D-12 for 804 800.

E= -1658.67686405615

DIIS: error= 3.85D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67686405615 IErMin= 1 ErrMin= 3.85D-04

ErrMax= 3.85D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.92D-04 BMatP= 3.92D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.85D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.428 Goal= None Shift= 0.000

Gap= 0.484 Goal= None Shift= 0.000

RMSDP=3.80D-05 MaxDP=9.57D-04 OVMax= 2.45D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.80D-05 CP: 1.00D+00

E= -1658.67701934620 Delta-E= -0.000155290055 Rises=F Damp=F

DIIS: error= 4.74D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67701934620 IErMin= 2 ErrMin= 4.74D-05

ErrMax= 4.74D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.24D-06 BMatP= 3.92D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.596D-01 0.106D+01

Coeff: -0.596D-01 0.106D+01

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.17D-06 MaxDP=1.49D-04 DE=-1.55D-04 OVMax= 3.20D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 5.54D-06 CP: 1.00D+00 1.07D+00

E= -1658.67702049623 Delta-E= -0.000001150029 Rises=F Damp=F

DIIS: error= 5.70D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67702049623 IErMin= 2 ErrMin= 4.74D-05

ErrMax= 5.70D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.41D-06 BMatP= 5.24D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.343D-01 0.509D+00 0.526D+00

Coeff: -0.343D-01 0.509D+00 0.526D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.98D-06 MaxDP=1.39D-04 DE=-1.15D-06 OVMax= 2.26D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.04D-06 CP: 1.00D+00 1.09D+00 6.22D-01

E= -1658.67702105616 Delta-E= -0.000000559930 Rises=F Damp=F

DIIS: error= 3.35D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67702105616 IErMin= 4 ErrMin= 3.35D-05

ErrMax= 3.35D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.52D-07 BMatP= 3.41D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.115D-01 0.153D+00 0.315D+00 0.543D+00

Coeff: -0.115D-01 0.153D+00 0.315D+00 0.543D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.15D-06 MaxDP=4.74D-05 DE=-5.60D-07 OVMax= 1.09D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 7.99D-07 CP: 1.00D+00 1.09D+00 7.07D-01 6.74D-01

E= -1658.67702116338 Delta-E= -0.000000107218 Rises=F Damp=F

DIIS: error= 1.00D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67702116338 IErMin= 5 ErrMin= 1.00D-05

ErrMax= 1.00D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.59D-08 BMatP= 6.52D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.410D-02 0.499D-01 0.150D+00 0.333D+00 0.472D+00

Coeff: -0.410D-02 0.499D-01 0.150D+00 0.333D+00 0.472D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.68D-07 MaxDP=1.69D-05 DE=-1.07D-07 OVMax= 3.40D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.54D-07 CP: 1.00D+00 1.09D+00 7.14D-01 7.41D-01 7.18D-01

E= -1658.67702117737 Delta-E= -0.000000013986 Rises=F Damp=F

DIIS: error= 1.92D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67702117737 IErMin= 6 ErrMin= 1.92D-06

ErrMax= 1.92D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.93D-09 BMatP= 7.59D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.725D-04-0.490D-02 0.162D-01 0.669D-01 0.244D+00 0.678D+00

Coeff: 0.725D-04-0.490D-02 0.162D-01 0.669D-01 0.244D+00 0.678D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.43D-07 MaxDP=9.80D-06 DE=-1.40D-08 OVMax= 1.04D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.05D-07 CP: 1.00D+00 1.09D+00 7.27D-01 7.50D-01 7.76D-01

CP: 8.40D-01

E= -1658.67702117842 Delta-E= -0.000000001048 Rises=F Damp=F

DIIS: error= 5.92D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67702117842 IErMin= 7 ErrMin= 5.92D-07

ErrMax= 5.92D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.60D-10 BMatP= 5.93D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.359D-03-0.658D-02-0.323D-02 0.854D-02 0.875D-01 0.347D+00

Coeff-Com: 0.566D+00

Coeff: 0.359D-03-0.658D-02-0.323D-02 0.854D-02 0.875D-01 0.347D+00

Coeff: 0.566D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.69D-08 MaxDP=2.02D-06 DE=-1.05D-09 OVMax= 5.36D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 4.57D-08 CP: 1.00D+00 1.09D+00 7.26D-01 7.56D-01 8.08D-01

CP: 8.96D-01 9.23D-01

E= -1658.67702117862 Delta-E= -0.000000000206 Rises=F Damp=F

DIIS: error= 1.66D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67702117862 IErMin= 8 ErrMin= 1.66D-07

ErrMax= 1.66D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.01D-11 BMatP= 6.60D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.127D-03-0.189D-02-0.338D-02-0.533D-02 0.304D-02 0.473D-01

Coeff-Com: 0.234D+00 0.726D+00

Coeff: 0.127D-03-0.189D-02-0.338D-02-0.533D-02 0.304D-02 0.473D-01

Coeff: 0.234D+00 0.726D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.72D-08 MaxDP=9.49D-07 DE=-2.06D-10 OVMax= 2.94D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.62D-08 CP: 1.00D+00 1.09D+00 7.27D-01 7.57D-01 8.17D-01

CP: 9.40D-01 1.07D+00 1.03D+00

E= -1658.67702117864 Delta-E= -0.000000000014 Rises=F Damp=F

DIIS: error= 7.55D-08 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67702117864 IErMin= 9 ErrMin= 7.55D-08

ErrMax= 7.55D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.87D-11 BMatP= 6.01D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.381D-05 0.209D-03-0.127D-02-0.456D-02-0.151D-01-0.393D-01

Coeff-Com: 0.235D-01 0.398D+00 0.639D+00

Coeff: 0.381D-05 0.209D-03-0.127D-02-0.456D-02-0.151D-01-0.393D-01

Coeff: 0.235D-01 0.398D+00 0.639D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.63D-08 MaxDP=6.19D-07 DE=-1.41D-11 OVMax= 2.01D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 7.39D-09 CP: 1.00D+00 1.09D+00 7.28D-01 7.58D-01 8.24D-01

CP: 9.53D-01 1.15D+00 1.24D+00 9.05D-01

E= -1658.67702117863 Delta-E= 0.000000000005 Rises=F Damp=F

DIIS: error= 5.20D-08 at cycle 10 NSaved= 10.

NSaved=10 IEnMin= 9 EnMin= -1658.67702117864 IErMin=10 ErrMin= 5.20D-08

ErrMax= 5.20D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.38D-12 BMatP= 1.87D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.291D-04 0.607D-03 0.656D-04-0.143D-02-0.995D-02-0.361D-01

Coeff-Com: -0.467D-01 0.594D-01 0.371D+00 0.663D+00

Coeff: -0.291D-04 0.607D-03 0.656D-04-0.143D-02-0.995D-02-0.361D-01

Coeff: -0.467D-01 0.594D-01 0.371D+00 0.663D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=7.65D-09 MaxDP=3.37D-07 DE= 4.55D-12 OVMax= 8.21D-07

Error on total polarization charges = 0.04162

SCF Done: E(UB3LYP) = -1658.67702118 A.U. after 10 cycles

NFock= 10 Conv=0.77D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655233541508D+03 PE=-6.147195615853D+03 EE= 1.731067593231D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.63

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 18:00:06 2019, MaxMem= 1342177280 cpu: 258.3

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 336

Leave Link 701 at Sat Aug 17 18:00:07 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 18:00:07 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 18:00:11 2019, MaxMem= 1342177280 cpu: 38.4

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.42067911D+00-2.95909377D+00 6.29501061D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000057743 0.000018777 -0.000074885

2 6 -0.000002124 0.000013712 0.000029451

3 8 0.000058070 -0.000043504 0.000071356

4 8 -0.000049287 0.000062391 -0.000082139

5 6 0.000026525 -0.000017378 0.000014516

6 16 0.000063568 0.000034500 0.000037796

7 6 -0.000034127 0.000044701 0.000042764

8 16 -0.000044311 0.000000192 -0.000005990

9 16 -0.000043853 -0.000082625 0.000027405

10 6 0.000074634 0.000054552 0.000059597

11 6 -0.000011390 0.000033798 -0.000007797

12 6 -0.000037999 0.000041416 0.000002264

13 6 0.000056490 -0.000020513 -0.000015428

14 1 0.000029281 -0.000058653 0.000118252

15 1 0.000018217 0.000022322 0.000003312

16 1 -0.000021050 -0.000031343 -0.000034270

17 1 0.000029597 -0.000057103 -0.000035710

18 1 0.000000290 0.000018829 -0.000041994

19 1 -0.000003557 -0.000013506 0.000046309

20 1 -0.000014705 -0.000057608 -0.000001872

21 1 0.000024802 -0.000021424 -0.000075262

22 1 -0.000026878 0.000040584 -0.000003531

23 1 0.000011931 0.000000305 0.000051837

24 1 -0.000003385 -0.000025640 0.000001338

25 1 -0.000022703 -0.000013361 -0.000029459

26 1 -0.000008836 0.000011164 -0.000077952

27 1 -0.000011456 0.000045415 -0.000019909

-------------------------------------------------------------------

Cartesian Forces: Max 0.000118252 RMS 0.000041092

Leave Link 716 at Sat Aug 17 18:00:11 2019, MaxMem= 1342177280 cpu: 0.3

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000205192 RMS 0.000037805

Search for a local minimum.

Step number 65 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .37805D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43 45 44 47 46

49 48 51 50 53

54 55 56 52 57

59 60 61 62 63

64 65

DE= 1.45D-05 DEPred=-3.38D-06 R=-4.28D+00

Trust test=-4.28D+00 RLast= 2.25D-02 DXMaxT set to 6.43D-02

ITU= -1 1 1 1 -1 1 0 -1 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 1 1 1 1 1 -1 -1 0 -1 -1 -1 0 -1 0 0 -1 -1 0 0

ITU= -1 0 0 -1 1 -1 1 -1 1 1 -1 1 -1 1 1 -1 0 0 -1 0

ITU= 0 -1 -1 0 0

Eigenvalues --- 0.00074 0.00153 0.00225 0.00268 0.00301

Eigenvalues --- 0.00340 0.00526 0.00912 0.01666 0.01942

Eigenvalues --- 0.03053 0.03521 0.03568 0.03866 0.04549

Eigenvalues --- 0.04696 0.04790 0.04816 0.05017 0.05235

Eigenvalues --- 0.05383 0.05464 0.05597 0.05724 0.08051

Eigenvalues --- 0.08308 0.08414 0.10891 0.11030 0.11503

Eigenvalues --- 0.12100 0.13365 0.14816 0.15275 0.15631

Eigenvalues --- 0.16056 0.16235 0.16361 0.17021 0.17584

Eigenvalues --- 0.18695 0.19070 0.20427 0.21650 0.22325

Eigenvalues --- 0.22386 0.23501 0.24546 0.25602 0.26596

Eigenvalues --- 0.27786 0.28819 0.29258 0.29701 0.30582

Eigenvalues --- 0.31317 0.33063 0.33615 0.33863 0.33883

Eigenvalues --- 0.33931 0.34001 0.34043 0.34066 0.34109

Eigenvalues --- 0.34204 0.34297 0.34431 0.35014 0.35586

Eigenvalues --- 0.36828 0.38495 0.48852 0.53353 0.86095

En-DIIS/RFO-DIIS IScMMF= 0 using points: 65 64 63 62 61

RFO step: Lambda=-3.68299417D-07.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 1.50D-05 SmlDif= 1.00D-05

RMS Error= 0.9492275259D-04 NUsed= 5 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.47693 0.08680 0.40108 0.04091 -0.00572

Iteration 1 RMS(Cart)= 0.00262983 RMS(Int)= 0.00000231

Iteration 2 RMS(Cart)= 0.00000642 RMS(Int)= 0.00000005

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000005

ITry= 1 IFail=0 DXMaxC= 1.06D-02 DCOld= 1.00D+10 DXMaxT= 6.43D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83556 0.00005 0.00009 0.00009 0.00018 2.83574

R2 2.28947 -0.00010 -0.00017 0.00002 -0.00015 2.28932

R3 2.55341 -0.00004 -0.00002 0.00005 0.00003 2.55344

R4 2.86553 -0.00007 -0.00017 -0.00005 -0.00022 2.86531

R5 3.61100 -0.00003 -0.00031 0.00066 0.00036 3.61135

R6 2.05796 -0.00002 -0.00001 -0.00001 -0.00002 2.05794

R7 1.83692 -0.00004 -0.00002 -0.00004 -0.00005 1.83686

R8 2.06137 -0.00003 -0.00007 -0.00003 -0.00010 2.06127

R9 2.06882 -0.00004 -0.00008 -0.00004 -0.00012 2.06869

R10 2.06012 -0.00004 -0.00002 -0.00004 -0.00006 2.06006

R11 3.31547 -0.00009 -0.00007 -0.00034 -0.00040 3.31506

R12 3.38819 0.00000 -0.00007 0.00014 0.00007 3.38826

R13 3.25400 -0.00008 -0.00018 -0.00015 -0.00032 3.25368

R14 3.47183 0.00003 0.00015 0.00000 0.00015 3.47199

R15 2.88161 -0.00003 -0.00010 -0.00003 -0.00013 2.88148

R16 2.06445 -0.00004 -0.00010 0.00002 -0.00008 2.06438

R17 2.06022 -0.00005 -0.00008 -0.00005 -0.00013 2.06009

R18 2.89421 -0.00001 -0.00004 -0.00001 -0.00005 2.89415

R19 2.07225 -0.00003 -0.00005 -0.00002 -0.00007 2.07218

R20 2.07128 -0.00003 -0.00007 0.00002 -0.00005 2.07122

R21 2.88621 0.00002 0.00003 0.00010 0.00013 2.88633

R22 2.07205 -0.00004 -0.00008 -0.00002 -0.00010 2.07195

R23 2.07186 -0.00002 -0.00004 -0.00002 -0.00006 2.07181

R24 2.06773 -0.00003 -0.00005 -0.00002 -0.00007 2.06766

R25 2.06938 -0.00004 -0.00009 -0.00002 -0.00011 2.06927

R26 2.06912 -0.00003 -0.00004 -0.00001 -0.00006 2.06907

A1 2.17670 0.00000 -0.00004 -0.00012 -0.00017 2.17653

A2 1.97657 0.00003 0.00017 -0.00006 0.00011 1.97668

A3 2.12934 -0.00003 -0.00012 0.00020 0.00008 2.12942

A4 2.02551 0.00009 0.00050 0.00005 0.00055 2.02606

A5 1.83104 0.00002 -0.00006 -0.00003 -0.00010 1.83095

A6 1.87276 0.00001 0.00030 -0.00017 0.00013 1.87290

A7 1.94711 -0.00010 -0.00039 0.00010 -0.00029 1.94682

A8 1.94197 -0.00006 -0.00023 -0.00027 -0.00050 1.94148

A9 1.83210 0.00006 -0.00016 0.00037 0.00021 1.83231

A10 1.87287 0.00003 -0.00006 0.00009 0.00003 1.87290

A11 1.91339 -0.00006 -0.00025 0.00004 -0.00020 1.91319

A12 1.92597 0.00002 0.00028 -0.00021 0.00006 1.92604

A13 1.95236 -0.00002 -0.00010 0.00001 -0.00008 1.95228

A14 1.88334 0.00002 0.00006 -0.00003 0.00003 1.88337

A15 1.89423 0.00003 -0.00006 0.00012 0.00006 1.89429

A16 1.89293 0.00001 0.00008 0.00007 0.00014 1.89307

A17 1.79905 -0.00021 -0.00035 -0.00024 -0.00060 1.79845

A18 1.96912 -0.00003 0.00011 0.00014 0.00025 1.96936

A19 2.14355 -0.00005 -0.00012 -0.00029 -0.00041 2.14314

A20 2.15533 0.00007 0.00011 -0.00016 -0.00006 2.15527

A21 1.79634 0.00008 -0.00007 0.00014 0.00006 1.79640

A22 1.92608 -0.00001 0.00012 -0.00021 -0.00008 1.92600

A23 1.88028 0.00000 -0.00031 0.00011 -0.00020 1.88008

A24 1.89148 0.00000 0.00017 -0.00018 -0.00002 1.89146

A25 1.93944 -0.00002 -0.00008 -0.00020 -0.00029 1.93915

A26 1.93802 0.00003 0.00005 0.00024 0.00029 1.93830

A27 1.88669 0.00001 0.00004 0.00026 0.00030 1.88698

A28 1.95304 0.00002 0.00003 0.00014 0.00017 1.95321

A29 1.91552 0.00002 0.00024 0.00002 0.00026 1.91578

A30 1.91753 -0.00003 -0.00018 -0.00004 -0.00022 1.91730

A31 1.90688 -0.00002 -0.00002 0.00007 0.00005 1.90692

A32 1.90840 0.00001 0.00004 -0.00003 0.00001 1.90841

A33 1.86011 -0.00001 -0.00011 -0.00017 -0.00028 1.85983

A34 1.96599 -0.00002 0.00001 -0.00018 -0.00017 1.96582

A35 1.90629 0.00001 0.00001 0.00014 0.00015 1.90644

A36 1.90772 0.00001 0.00002 0.00005 0.00008 1.90779

A37 1.91299 -0.00001 -0.00008 0.00002 -0.00006 1.91292

A38 1.91271 0.00001 0.00008 -0.00003 0.00006 1.91276

A39 1.85483 0.00000 -0.00005 0.00000 -0.00005 1.85478

A40 1.94538 0.00002 0.00006 0.00014 0.00021 1.94559

A41 1.94211 -0.00001 0.00001 0.00005 0.00006 1.94217

A42 1.94280 -0.00001 -0.00001 -0.00019 -0.00021 1.94259

A43 1.87696 0.00001 0.00001 0.00006 0.00007 1.87702

A44 1.87722 0.00000 -0.00006 -0.00005 -0.00011 1.87711

A45 1.87599 0.00001 -0.00001 -0.00001 -0.00001 1.87598

D1 2.68646 0.00001 0.00655 -0.00321 0.00334 2.68980

D2 -1.43936 -0.00005 0.00633 -0.00308 0.00324 -1.43612

D3 0.50287 0.00003 0.00625 -0.00275 0.00349 0.50636

D4 -0.49124 0.00002 0.00663 -0.00279 0.00384 -0.48740

D5 1.66612 -0.00004 0.00641 -0.00266 0.00375 1.66987

D6 -2.67483 0.00004 0.00633 -0.00233 0.00400 -2.67083

D7 -3.09933 -0.00003 -0.00049 -0.00120 -0.00169 -3.10103

D8 0.00726 -0.00001 -0.00041 -0.00080 -0.00121 0.00605

D9 3.14026 -0.00001 -0.00003 -0.00025 -0.00028 3.13998

D10 -1.07094 -0.00001 0.00006 -0.00039 -0.00033 -1.07127

D11 1.03813 0.00001 0.00028 -0.00044 -0.00017 1.03797

D12 1.04452 -0.00002 -0.00001 -0.00032 -0.00033 1.04420

D13 3.11652 -0.00002 0.00008 -0.00046 -0.00038 3.11614

D14 -1.05760 0.00000 0.00030 -0.00051 -0.00021 -1.05781

D15 -0.99514 0.00001 0.00058 -0.00066 -0.00009 -0.99522

D16 1.07686 0.00002 0.00067 -0.00081 -0.00014 1.07672

D17 -3.09726 0.00003 0.00089 -0.00086 0.00003 -3.09723

D18 -3.08767 0.00001 -0.00106 0.00085 -0.00020 -3.08787

D19 -0.88093 0.00007 -0.00072 0.00095 0.00023 -0.88071

D20 1.22432 -0.00003 -0.00130 0.00090 -0.00040 1.22392

D21 1.82028 -0.00006 0.00048 -0.00158 -0.00109 1.81918

D22 -1.14067 0.00000 -0.00010 0.00028 0.00019 -1.14048

D23 2.59770 0.00004 -0.00097 0.00220 0.00123 2.59893

D24 -0.72594 -0.00003 -0.00042 0.00032 -0.00011 -0.72605

D25 -3.03877 0.00004 0.00087 0.00284 0.00371 -3.03505

D26 -0.91858 0.00000 0.00065 0.00254 0.00319 -0.91539

D27 1.11885 0.00001 0.00062 0.00280 0.00342 1.12228

D28 -3.12329 -0.00002 -0.00058 -0.00162 -0.00220 -3.12550

D29 -1.00329 -0.00001 -0.00042 -0.00143 -0.00185 -1.00514

D30 1.03657 -0.00002 -0.00053 -0.00164 -0.00217 1.03440

D31 1.07519 0.00001 -0.00022 -0.00149 -0.00171 1.07347

D32 -3.08800 0.00002 -0.00006 -0.00129 -0.00136 -3.08936

D33 -1.04814 0.00000 -0.00017 -0.00151 -0.00168 -1.04982

D34 -1.02549 -0.00001 -0.00026 -0.00184 -0.00209 -1.02758

D35 1.09452 0.00000 -0.00010 -0.00164 -0.00174 1.09278

D36 3.13437 -0.00001 -0.00020 -0.00186 -0.00206 3.13232

D37 -3.13260 0.00002 0.00010 -0.00039 -0.00030 -3.13289

D38 -1.00263 0.00001 0.00000 -0.00039 -0.00038 -1.00301

D39 1.01996 0.00001 -0.00003 -0.00028 -0.00031 1.01965

D40 1.02561 -0.00001 -0.00021 -0.00056 -0.00077 1.02485

D41 -3.12761 -0.00002 -0.00030 -0.00055 -0.00085 -3.12846

D42 -1.10501 -0.00001 -0.00034 -0.00044 -0.00078 -1.10579

D43 -1.00403 0.00000 -0.00009 -0.00038 -0.00046 -1.00449

D44 1.12594 -0.00001 -0.00018 -0.00037 -0.00055 1.12539

D45 -3.13466 0.00000 -0.00021 -0.00026 -0.00048 -3.13513

D46 3.13882 -0.00001 -0.00023 -0.00073 -0.00096 3.13786

D47 -1.04925 0.00000 -0.00017 -0.00052 -0.00070 -1.04995

D48 1.04290 -0.00001 -0.00019 -0.00063 -0.00082 1.04208

D49 1.01264 -0.00001 -0.00019 -0.00080 -0.00099 1.01165

D50 3.10776 0.00000 -0.00014 -0.00060 -0.00073 3.10703

D51 -1.08328 -0.00001 -0.00015 -0.00070 -0.00085 -1.08413

D52 -1.01656 -0.00001 -0.00014 -0.00080 -0.00094 -1.01750

D53 1.07856 0.00000 -0.00008 -0.00060 -0.00068 1.07788

D54 -3.11248 -0.00001 -0.00009 -0.00070 -0.00079 -3.11327

Item Value Threshold Converged?

Maximum Force 0.000205 0.000450 YES

RMS Force 0.000038 0.000300 YES

Maximum Displacement 0.010611 0.001800 NO

RMS Displacement 0.002629 0.001200 NO

Predicted change in Energy=-5.611319D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 18:00:11 2019, MaxMem= 1342177280 cpu: 0.6

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.097023 -0.406723 -0.196306

2 6 0 -2.843515 0.074317 0.473875

3 8 0 -4.908262 0.311151 -0.738684

4 8 0 -4.227910 -1.751503 -0.180806

5 6 0 -2.292624 -0.812926 1.573128

6 16 0 -1.582807 0.298904 -0.944671

7 6 0 -0.118549 0.771289 -0.101930

8 16 0 1.080276 -0.557416 0.008403

9 16 0 0.021585 2.251750 0.765886

10 6 0 2.685994 0.335365 -0.008036

11 6 0 3.843109 -0.655627 -0.071806

12 6 0 5.201836 0.051024 -0.064374

13 6 0 6.373107 -0.926367 -0.140069

14 1 0 -3.037818 1.081389 0.839944

15 1 0 -5.042017 -1.968450 -0.665574

16 1 0 -1.385801 -0.366988 1.983752

17 1 0 -3.019363 -0.907318 2.386341

18 1 0 -2.052669 -1.811268 1.206894

19 1 0 2.688433 0.999294 -0.875546

20 1 0 2.746269 0.950633 0.889877

21 1 0 3.788930 -1.344274 0.779811

22 1 0 3.758087 -1.269468 -0.975844

23 1 0 5.250335 0.749334 -0.908276

24 1 0 5.288951 0.659652 0.843356

25 1 0 7.333332 -0.401825 -0.137325

26 1 0 6.371074 -1.615676 0.710751

27 1 0 6.329200 -1.529911 -1.052549

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.500608 0.000000

3 O 1.211455 2.406152 0.000000

4 O 1.351224 2.383018 2.242464 0.000000

5 C 2.559639 1.516257 3.667367 2.775346 0.000000

6 S 2.716476 1.911046 3.331851 3.432817 2.842414

7 C 4.150286 2.871021 4.853714 4.822609 3.168937

8 S 5.183536 4.001486 6.097142 5.444124 3.726944

9 S 4.995620 3.610441 5.507544 5.914429 3.924212

10 C 6.826086 5.556604 7.629361 7.224053 5.348391

11 C 7.945008 6.748446 8.829829 8.145808 6.354351

12 C 9.311054 8.063370 10.135899 9.601187 7.719764

13 C 10.483168 9.291093 11.364817 10.633160 8.834184

14 H 2.100049 1.089016 2.565910 3.237828 2.163631

15 H 1.884733 3.210086 2.284691 0.972027 3.729100

16 H 3.479217 2.144623 4.503249 3.831419 1.090779

17 H 2.842888 2.156863 3.849466 2.960317 1.094704

18 H 2.849754 2.172138 4.055162 2.580883 1.090135

19 H 6.962806 5.768793 7.629027 7.475651 5.838757

20 H 7.060656 5.673330 7.851942 7.555599 5.382139

21 H 8.001253 6.789353 8.982616 8.084451 6.156052

22 H 7.940702 6.891196 8.812502 8.039937 6.581549

23 H 9.445447 8.238713 10.169457 9.829574 8.092852

24 H 9.503397 8.161870 10.325088 9.870827 7.757663

25 H 11.430508 10.206296 12.277075 11.639838 9.785381

26 H 10.576643 9.371277 11.534164 10.637283 8.743441

27 H 10.521446 9.436218 11.391601 10.595358 9.041244

6 7 8 9 10

6 S 0.000000

7 C 1.754256 0.000000

8 S 2.955275 1.792990 0.000000

9 S 3.051833 1.721774 3.096131 0.000000

10 C 4.370501 2.839772 1.837296 3.372026 0.000000

11 C 5.577956 4.210906 2.765741 4.874282 1.524811

12 C 6.846003 5.369049 4.166864 5.689247 2.532487

13 C 8.089824 6.710073 5.307751 7.159820 3.899257

14 H 2.431911 3.083086 4.509528 3.276457 5.834179

15 H 4.145470 5.662544 6.318840 6.745312 8.090864

16 H 3.009632 2.692893 3.165408 3.212744 4.586942

17 H 3.822867 4.174200 4.752270 4.674714 6.310975

18 H 3.050053 3.481873 3.581043 4.583136 5.342191

19 H 4.328836 2.920551 2.406425 3.372688 1.092421

20 H 4.746707 3.036944 2.413864 3.021951 1.090154

21 H 5.876175 4.530062 2.924212 5.208116 2.158323

22 H 5.566499 4.467294 2.940480 5.421628 2.159057

23 H 6.848069 5.429142 4.465118 5.692091 2.749118

24 H 7.109729 5.490636 4.459971 5.503265 2.757792

25 H 8.979998 7.543737 6.256688 7.830638 4.707220

26 H 8.346872 6.962274 5.441116 7.434786 4.231198

27 H 8.121333 6.911777 5.442661 7.575861 4.224123

11 12 13 14 15

11 C 0.000000

12 C 1.531519 0.000000

13 C 2.545358 1.527383 0.000000

14 H 7.155115 8.352924 9.672488 0.000000

15 H 9.001197 10.458310 11.474631 3.947774 0.000000

16 H 5.625846 6.911333 8.063757 2.476944 4.790775

17 H 7.293790 8.632065 9.726336 2.519254 3.811996

18 H 6.142538 7.596848 8.578523 3.077765 3.530870

19 H 2.172105 2.806138 4.222075 5.978260 8.283204

20 H 2.169784 2.783828 4.211635 5.785780 8.461553

21 H 1.096550 2.157733 2.774671 7.245132 8.970193

22 H 1.096044 2.158446 2.766689 7.416733 8.833271

23 H 2.157286 1.096430 2.158410 8.477028 10.647900

24 H 2.158226 1.096353 2.158234 8.337442 10.766276

25 H 3.500051 2.180290 1.094158 10.522154 12.485296

26 H 2.815083 2.178491 1.095010 9.788672 11.501190

27 H 2.811916 2.178714 1.094903 9.906636 11.386248

16 17 18 19 20

16 H 0.000000

17 H 1.767076 0.000000

18 H 1.770357 1.772772 0.000000

19 H 5.161560 6.845000 5.891847 0.000000

20 H 4.472885 6.239704 5.546026 1.767041 0.000000

21 H 5.402074 7.008903 5.875777 3.073046 2.523064

22 H 6.002771 7.574250 6.230792 2.510279 3.071406

23 H 7.324500 9.054662 8.022748 2.574275 3.089372

24 H 6.848855 8.594433 7.754804 3.135709 2.559700

25 H 8.973487 10.667835 9.585951 4.907462 4.891362

26 H 7.959200 9.565024 8.440608 4.787092 4.444911

27 H 8.372142 9.980442 8.685618 4.436596 4.771112

21 22 23 24 25

21 H 0.000000

22 H 1.757519 0.000000

23 H 3.060807 2.511361 0.000000

24 H 2.503961 3.061787 1.754352 0.000000

25 H 3.780494 3.773367 2.501681 2.503590 0.000000

26 H 2.597287 3.129244 3.077430 2.523032 1.765958

27 H 3.137671 2.585408 2.525811 3.077460 1.765926

26 27

26 H 0.000000

27 H 1.765881 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.25D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.104505 -0.465836 -0.121380

2 6 0 -2.846110 0.116722 0.452113

3 8 0 -4.919668 0.154744 -0.767919

4 8 0 -4.235319 -1.789841 0.114633

5 6 0 -2.287218 -0.579622 1.677584

6 16 0 -1.595811 0.104915 -0.993123

7 6 0 -0.125408 0.706877 -0.249502

8 16 0 1.074149 -0.587405 0.067845

9 16 0 0.021120 2.309084 0.363661

10 6 0 2.679732 0.288715 -0.105864

11 6 0 3.836318 -0.700796 -0.015166

12 6 0 5.195086 -0.004100 -0.133125

13 6 0 6.365740 -0.982158 -0.056516

14 1 0 -3.037696 1.170318 0.650067

15 1 0 -5.052958 -2.082095 -0.322275

16 1 0 -1.377400 -0.073688 2.003255

17 1 0 -3.007989 -0.538954 2.500513

18 1 0 -2.049981 -1.624689 1.477712

19 1 0 2.675844 0.801941 -1.070211

20 1 0 2.746597 1.042378 0.678965

21 1 0 3.788350 -1.240942 0.937915

22 1 0 3.744662 -1.454022 -0.806092

23 1 0 5.237429 0.546847 -1.080133

24 1 0 5.288861 0.744584 0.662280

25 1 0 7.325976 -0.465399 -0.146463

26 1 0 6.369911 -1.523151 0.895511

27 1 0 6.315136 -1.726656 -0.857750

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3046924 0.1935357 0.1808696

Leave Link 202 at Sat Aug 17 18:00:11 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.3517366370 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0550022331 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.2967344039 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2320

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.11D-07

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 91

GePol: Fraction of low-weight points (<1% of avg) = 3.92%

GePol: Cavity surface area = 309.307 Ang\*\*2

GePol: Cavity volume = 320.447 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057897271 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.2909446768 Hartrees.

Leave Link 301 at Sat Aug 17 18:00:11 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 18:00:11 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 18:00:11 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000114 -0.000004 -0.000017 Ang= -0.01 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 18:00:11 2019, MaxMem= 1342177280 cpu: 2.7

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16147200.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.33D-15 for 2320.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.77D-15 for 587 305.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.77D-15 for 2314.

Iteration 1 A^-1\*A deviation from orthogonality is 7.73D-10 for 2129 895.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.66D-15 for 434.

Iteration 2 A\*A^-1 deviation from orthogonality is 2.22D-15 for 798 122.

Iteration 2 A^-1\*A deviation from unit magnitude is 9.99D-16 for 397.

Iteration 2 A^-1\*A deviation from orthogonality is 4.31D-16 for 365 345.

E= -1658.67700651727

DIIS: error= 1.84D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67700651727 IErMin= 1 ErrMin= 1.84D-04

ErrMax= 1.84D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.84D-05 BMatP= 3.84D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.84D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.428 Goal= None Shift= 0.000

Gap= 0.484 Goal= None Shift= 0.000

RMSDP=1.42D-05 MaxDP=3.46D-04 OVMax= 8.43D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.42D-05 CP: 1.00D+00

E= -1658.67702385754 Delta-E= -0.000017340267 Rises=F Damp=F

DIIS: error= 2.78D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67702385754 IErMin= 2 ErrMin= 2.78D-05

ErrMax= 2.78D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.74D-07 BMatP= 3.84D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.576D-01 0.106D+01

Coeff: -0.576D-01 0.106D+01

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.88D-06 MaxDP=1.06D-04 DE=-1.73D-05 OVMax= 2.66D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.72D-06 CP: 1.00D+00 1.07D+00

E= -1658.67702390924 Delta-E= -0.000000051700 Rises=F Damp=F

DIIS: error= 2.20D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67702390924 IErMin= 3 ErrMin= 2.20D-05

ErrMax= 2.20D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.39D-07 BMatP= 7.74D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.422D-01 0.591D+00 0.451D+00

Coeff: -0.422D-01 0.591D+00 0.451D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.07D-06 MaxDP=1.03D-04 DE=-5.17D-08 OVMax= 2.14D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.20D-06 CP: 1.00D+00 1.09D+00 3.94D-01

E= -1658.67702409806 Delta-E= -0.000000188822 Rises=F Damp=F

DIIS: error= 9.63D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67702409806 IErMin= 4 ErrMin= 9.63D-06

ErrMax= 9.63D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.51D-07 BMatP= 7.74D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.127D-01 0.154D+00 0.292D+00 0.566D+00

Coeff: -0.127D-01 0.154D+00 0.292D+00 0.566D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.68D-07 MaxDP=3.07D-05 DE=-1.89D-07 OVMax= 7.58D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.86D-07 CP: 1.00D+00 1.09D+00 5.70D-01 6.98D-01

E= -1658.67702413419 Delta-E= -0.000000036129 Rises=F Damp=F

DIIS: error= 1.19D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67702413419 IErMin= 5 ErrMin= 1.19D-06

ErrMax= 1.19D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.04D-09 BMatP= 1.51D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.263D-02 0.260D-01 0.861D-01 0.216D+00 0.674D+00

Coeff: -0.263D-02 0.260D-01 0.861D-01 0.216D+00 0.674D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.17D-07 MaxDP=4.78D-06 DE=-3.61D-08 OVMax= 1.07D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 8.60D-08 CP: 1.00D+00 1.09D+00 5.81D-01 7.50D-01 8.81D-01

E= -1658.67702413490 Delta-E= -0.000000000708 Rises=F Damp=F

DIIS: error= 8.68D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67702413490 IErMin= 6 ErrMin= 8.68D-07

ErrMax= 8.68D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.68D-10 BMatP= 3.04D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.554D-03-0.113D-01 0.537D-03 0.292D-01 0.359D+00 0.622D+00

Coeff: 0.554D-03-0.113D-01 0.537D-03 0.292D-01 0.359D+00 0.622D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.47D-08 MaxDP=1.60D-06 DE=-7.08D-10 OVMax= 6.19D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 4.17D-08 CP: 1.00D+00 1.09D+00 5.84D-01 7.69D-01 9.56D-01

CP: 8.57D-01

E= -1658.67702413507 Delta-E= -0.000000000172 Rises=F Damp=F

DIIS: error= 6.06D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67702413507 IErMin= 7 ErrMin= 6.06D-07

ErrMax= 6.06D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.91D-10 BMatP= 7.68D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.630D-03-0.101D-01-0.929D-02-0.534D-02 0.153D+00 0.399D+00

Coeff-Com: 0.472D+00

Coeff: 0.630D-03-0.101D-01-0.929D-02-0.534D-02 0.153D+00 0.399D+00

Coeff: 0.472D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.57D-08 MaxDP=8.40D-07 DE=-1.72D-10 OVMax= 2.75D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.72D-08 CP: 1.00D+00 1.09D+00 5.88D-01 7.68D-01 9.90D-01

CP: 9.69D-01 8.20D-01

E= -1658.67702413509 Delta-E= -0.000000000015 Rises=F Damp=F

DIIS: error= 1.28D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67702413509 IErMin= 8 ErrMin= 1.28D-07

ErrMax= 1.28D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.58D-11 BMatP= 1.91D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.172D-03-0.216D-02-0.457D-02-0.870D-02-0.670D-02 0.523D-01

Coeff-Com: 0.229D+00 0.741D+00

Coeff: 0.172D-03-0.216D-02-0.457D-02-0.870D-02-0.670D-02 0.523D-01

Coeff: 0.229D+00 0.741D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.25D-08 MaxDP=4.56D-07 DE=-1.55D-11 OVMax= 2.23D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 7.00D-09 CP: 1.00D+00 1.09D+00 5.88D-01 7.71D-01 1.01D+00

CP: 1.04D+00 9.51D-01 9.89D-01

E= -1658.67702413509 Delta-E= -0.000000000002 Rises=F Damp=F

DIIS: error= 3.17D-08 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67702413509 IErMin= 9 ErrMin= 3.17D-08

ErrMax= 3.17D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.92D-12 BMatP= 1.58D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.470D-04 0.108D-02-0.133D-03-0.251D-02-0.313D-01-0.538D-01

Coeff-Com: 0.412D-02 0.293D+00 0.789D+00

Coeff: -0.470D-04 0.108D-02-0.133D-03-0.251D-02-0.313D-01-0.538D-01

Coeff: 0.412D-02 0.293D+00 0.789D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.17D-09 MaxDP=2.60D-07 DE=-1.82D-12 OVMax= 1.19D-06

Error on total polarization charges = 0.04162

SCF Done: E(UB3LYP) = -1658.67702414 A.U. after 9 cycles

NFock= 9 Conv=0.62D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655235100427D+03 PE=-6.147345222696D+03 EE= 1.731142153457D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.63

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 18:00:32 2019, MaxMem= 1342177280 cpu: 240.2

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 336

Leave Link 701 at Sat Aug 17 18:00:33 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 18:00:33 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 18:00:37 2019, MaxMem= 1342177280 cpu: 37.5

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.42140763D+00-2.95803888D+00 6.32080966D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000043647 -0.000023331 0.000068894

2 6 -0.000033510 -0.000006162 -0.000048219

3 8 -0.000027210 0.000010795 0.000007764

4 8 -0.000022706 0.000074315 -0.000046572

5 6 0.000007374 -0.000052055 -0.000013444

6 16 -0.000013897 0.000007480 0.000058267

7 6 0.000030245 0.000014356 0.000056575

8 16 -0.000035268 0.000000094 -0.000034555

9 16 0.000005097 0.000004781 0.000065017

10 6 0.000023105 0.000005384 0.000021208

11 6 -0.000005560 0.000004828 -0.000019962

12 6 0.000010262 0.000001126 0.000030183

13 6 0.000003606 0.000015325 -0.000042778

14 1 0.000024778 -0.000019004 0.000056797

15 1 0.000008587 0.000023507 -0.000043635

16 1 -0.000001391 -0.000034050 -0.000010413

17 1 0.000003097 -0.000066890 -0.000008593

18 1 0.000005460 -0.000013046 -0.000031291

19 1 -0.000017715 0.000016163 0.000043304

20 1 0.000008207 -0.000013040 0.000015119

21 1 0.000014132 -0.000015986 -0.000037269

22 1 -0.000006923 0.000040445 -0.000028420

23 1 -0.000001648 0.000011705 0.000021869

24 1 -0.000002045 -0.000015421 0.000019272

25 1 -0.000009687 0.000010729 -0.000015635

26 1 -0.000008664 -0.000005790 -0.000048410

27 1 -0.000001372 0.000023742 -0.000035072

-------------------------------------------------------------------

Cartesian Forces: Max 0.000074315 RMS 0.000029168

Leave Link 716 at Sat Aug 17 18:00:37 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000059368 RMS 0.000014460

Search for a local minimum.

Step number 66 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .14460D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43 45 44 47 46

49 48 51 50 53

54 55 56 52 57

59 60 61 62 63

64 65 66

DE= -2.96D-06 DEPred=-5.61D-07 R= 5.27D+00

TightC=F SS= 1.41D+00 RLast= 1.29D-02 DXNew= 1.0812D-01 3.8708D-02

Trust test= 5.27D+00 RLast= 1.29D-02 DXMaxT set to 6.43D-02

ITU= 1 -1 1 1 1 -1 1 0 -1 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 1 1 1 1 1 -1 -1 0 -1 -1 -1 0 -1 0 0 -1 -1 0

ITU= 0 -1 0 0 -1 1 -1 1 -1 1 1 -1 1 -1 1 1 -1 0 0 -1

ITU= 0 0 -1 -1 0 0

Eigenvalues --- 0.00048 0.00155 0.00225 0.00270 0.00327

Eigenvalues --- 0.00334 0.00521 0.00950 0.01733 0.02019

Eigenvalues --- 0.03217 0.03532 0.03604 0.03877 0.04128

Eigenvalues --- 0.04507 0.04797 0.04810 0.04938 0.05251

Eigenvalues --- 0.05431 0.05472 0.05554 0.05725 0.07810

Eigenvalues --- 0.08302 0.08443 0.10252 0.11101 0.11234

Eigenvalues --- 0.12092 0.13366 0.14573 0.15226 0.15722

Eigenvalues --- 0.16046 0.16138 0.16275 0.17016 0.17384

Eigenvalues --- 0.18265 0.20195 0.20376 0.21450 0.22175

Eigenvalues --- 0.22531 0.23309 0.24209 0.25313 0.26322

Eigenvalues --- 0.27436 0.28559 0.29134 0.29483 0.30094

Eigenvalues --- 0.30800 0.32224 0.33525 0.33831 0.33861

Eigenvalues --- 0.33907 0.33961 0.34017 0.34053 0.34124

Eigenvalues --- 0.34202 0.34223 0.34298 0.34961 0.35029

Eigenvalues --- 0.36382 0.37366 0.47988 0.52601 0.79356

En-DIIS/RFO-DIIS IScMMF= 0 using points: 66 65 64 63 62

RFO step: Lambda=-6.06718709D-08.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 6.00D-06 SmlDif= 1.00D-05

RMS Error= 0.5164700268D-04 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 0.81306 0.16487 0.06046 -0.00393 -0.03446

Iteration 1 RMS(Cart)= 0.00268657 RMS(Int)= 0.00000541

Iteration 2 RMS(Cart)= 0.00000675 RMS(Int)= 0.00000002

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000002

ITry= 1 IFail=0 DXMaxC= 1.51D-02 DCOld= 1.00D+10 DXMaxT= 6.43D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83574 -0.00002 -0.00003 -0.00010 -0.00014 2.83560

R2 2.28932 0.00002 0.00001 0.00004 0.00005 2.28937

R3 2.55344 -0.00006 0.00000 -0.00011 -0.00011 2.55333

R4 2.86531 -0.00001 0.00003 0.00010 0.00014 2.86545

R5 3.61135 -0.00003 -0.00010 0.00014 0.00004 3.61140

R6 2.05794 0.00000 -0.00001 -0.00001 -0.00002 2.05792

R7 1.83686 0.00000 0.00000 -0.00005 -0.00004 1.83682

R8 2.06127 0.00000 0.00002 -0.00001 0.00001 2.06128

R9 2.06869 0.00000 0.00001 0.00001 0.00002 2.06871

R10 2.06006 -0.00001 0.00002 -0.00007 -0.00005 2.06001

R11 3.31506 0.00002 0.00004 -0.00001 0.00003 3.31509

R12 3.38826 -0.00001 0.00002 0.00001 0.00003 3.38829

R13 3.25368 0.00001 0.00001 -0.00001 0.00001 3.25369

R14 3.47199 0.00001 -0.00001 0.00003 0.00002 3.47201

R15 2.88148 0.00000 0.00000 0.00002 0.00002 2.88150

R16 2.06438 -0.00002 -0.00001 -0.00002 -0.00003 2.06435

R17 2.06009 -0.00001 0.00002 -0.00004 -0.00002 2.06007

R18 2.89415 -0.00001 0.00000 -0.00001 0.00000 2.89415

R19 2.07218 0.00000 0.00000 -0.00001 -0.00001 2.07217

R20 2.07122 -0.00001 -0.00001 0.00001 0.00000 2.07122

R21 2.88633 -0.00002 0.00000 -0.00004 -0.00004 2.88630

R22 2.07195 -0.00001 0.00000 -0.00001 -0.00001 2.07194

R23 2.07181 0.00000 0.00000 0.00000 0.00001 2.07181

R24 2.06766 -0.00001 0.00000 -0.00001 -0.00001 2.06765

R25 2.06927 -0.00001 0.00000 0.00000 -0.00001 2.06926

R26 2.06907 0.00000 0.00000 0.00000 0.00000 2.06907

A1 2.17653 0.00003 0.00008 0.00009 0.00017 2.17670

A2 1.97668 0.00002 -0.00008 -0.00004 -0.00012 1.97655

A3 2.12942 -0.00005 0.00000 -0.00005 -0.00005 2.12936

A4 2.02606 0.00001 -0.00009 -0.00020 -0.00029 2.02577

A5 1.83095 0.00001 0.00010 0.00023 0.00033 1.83128

A6 1.87290 0.00001 0.00000 0.00000 0.00000 1.87290

A7 1.94682 -0.00004 -0.00002 -0.00019 -0.00020 1.94662

A8 1.94148 -0.00001 0.00012 -0.00017 -0.00005 1.94142

A9 1.83231 0.00001 -0.00011 0.00040 0.00029 1.83260

A10 1.87290 0.00000 0.00002 0.00015 0.00017 1.87308

A11 1.91319 -0.00003 0.00005 -0.00024 -0.00020 1.91299

A12 1.92604 0.00001 0.00002 0.00004 0.00006 1.92610

A13 1.95228 0.00001 -0.00002 0.00007 0.00005 1.95232

A14 1.88337 0.00001 -0.00001 0.00010 0.00009 1.88346

A15 1.89429 0.00001 -0.00003 0.00000 -0.00003 1.89425

A16 1.89307 0.00000 -0.00001 0.00004 0.00003 1.89311

A17 1.79845 0.00005 0.00002 0.00013 0.00015 1.79860

A18 1.96936 -0.00004 -0.00005 -0.00032 -0.00038 1.96899

A19 2.14314 0.00002 0.00009 0.00009 0.00018 2.14332

A20 2.15527 0.00003 0.00002 0.00024 0.00026 2.15553

A21 1.79640 -0.00002 -0.00005 0.00028 0.00023 1.79663

A22 1.92600 0.00002 0.00001 -0.00001 -0.00001 1.92599

A23 1.88008 -0.00003 -0.00002 -0.00007 -0.00009 1.87999

A24 1.89146 0.00000 0.00009 -0.00002 0.00007 1.89153

A25 1.93915 0.00001 0.00003 -0.00008 -0.00005 1.93910

A26 1.93830 -0.00001 -0.00006 0.00018 0.00013 1.93843

A27 1.88698 0.00000 -0.00005 -0.00001 -0.00005 1.88693

A28 1.95321 -0.00001 0.00000 -0.00001 -0.00001 1.95321

A29 1.91578 0.00001 0.00000 0.00008 0.00008 1.91585

A30 1.91730 0.00000 -0.00002 -0.00002 -0.00005 1.91726

A31 1.90692 -0.00001 -0.00003 0.00000 -0.00003 1.90690

A32 1.90841 0.00001 0.00001 0.00001 0.00002 1.90843

A33 1.85983 0.00000 0.00004 -0.00006 -0.00002 1.85982

A34 1.96582 0.00001 0.00000 0.00002 0.00002 1.96584

A35 1.90644 -0.00001 -0.00004 0.00000 -0.00005 1.90639

A36 1.90779 0.00000 0.00002 -0.00002 0.00001 1.90780

A37 1.91292 0.00000 -0.00003 0.00000 -0.00003 1.91289

A38 1.91276 0.00000 0.00005 -0.00003 0.00001 1.91277

A39 1.85478 0.00000 0.00001 0.00004 0.00004 1.85482

A40 1.94559 -0.00001 -0.00002 -0.00001 -0.00003 1.94556

A41 1.94217 -0.00002 -0.00001 -0.00007 -0.00008 1.94209

A42 1.94259 0.00001 0.00000 0.00005 0.00005 1.94265

A43 1.87702 0.00001 0.00000 0.00006 0.00006 1.87709

A44 1.87711 0.00000 0.00001 0.00005 0.00005 1.87716

A45 1.87598 0.00000 0.00002 -0.00008 -0.00006 1.87592

D1 2.68980 0.00001 -0.00117 -0.00396 -0.00513 2.68467

D2 -1.43612 -0.00001 -0.00117 -0.00415 -0.00532 -1.44144

D3 0.50636 0.00001 -0.00126 -0.00359 -0.00485 0.50151

D4 -0.48740 0.00000 -0.00125 -0.00397 -0.00522 -0.49261

D5 1.66987 -0.00003 -0.00125 -0.00416 -0.00541 1.66446

D6 -2.67083 0.00000 -0.00134 -0.00360 -0.00494 -2.67577

D7 -3.10103 0.00002 0.00018 -0.00006 0.00012 -3.10091

D8 0.00605 0.00001 0.00011 -0.00006 0.00004 0.00609

D9 3.13998 0.00000 -0.00010 0.00140 0.00129 3.14127

D10 -1.07127 0.00000 -0.00008 0.00140 0.00132 -1.06995

D11 1.03797 0.00000 -0.00009 0.00152 0.00143 1.03940

D12 1.04420 0.00000 -0.00016 0.00138 0.00122 1.04542

D13 3.11614 0.00000 -0.00013 0.00138 0.00125 3.11739

D14 -1.05781 0.00000 -0.00014 0.00150 0.00136 -1.05645

D15 -0.99522 0.00001 -0.00008 0.00110 0.00102 -0.99420

D16 1.07672 0.00001 -0.00006 0.00110 0.00105 1.07777

D17 -3.09723 0.00002 -0.00006 0.00123 0.00116 -3.09607

D18 -3.08787 0.00000 -0.00049 0.00012 -0.00037 -3.08824

D19 -0.88071 0.00000 -0.00054 -0.00008 -0.00062 -0.88133

D20 1.22392 -0.00002 -0.00048 -0.00014 -0.00062 1.22330

D21 1.81918 -0.00001 0.00016 -0.00138 -0.00123 1.81796

D22 -1.14048 -0.00003 -0.00014 -0.00147 -0.00161 -1.14209

D23 2.59893 -0.00001 0.00018 0.00073 0.00091 2.59984

D24 -0.72605 0.00000 0.00048 0.00080 0.00129 -0.72476

D25 -3.03505 -0.00001 -0.00113 0.00033 -0.00081 -3.03586

D26 -0.91539 0.00000 -0.00111 0.00018 -0.00093 -0.91632

D27 1.12228 -0.00002 -0.00113 0.00012 -0.00100 1.12127

D28 -3.12550 -0.00001 0.00015 -0.00026 -0.00011 -3.12560

D29 -1.00514 -0.00001 0.00011 -0.00021 -0.00009 -1.00524

D30 1.03440 -0.00001 0.00015 -0.00025 -0.00010 1.03430

D31 1.07347 0.00000 0.00015 -0.00011 0.00004 1.07351

D32 -3.08936 0.00000 0.00011 -0.00006 0.00005 -3.08930

D33 -1.04982 0.00000 0.00015 -0.00010 0.00005 -1.04977

D34 -1.02758 0.00001 0.00023 -0.00017 0.00006 -1.02752

D35 1.09278 0.00000 0.00020 -0.00012 0.00007 1.09285

D36 3.13232 0.00001 0.00023 -0.00016 0.00007 3.13239

D37 -3.13289 0.00000 0.00020 -0.00096 -0.00076 -3.13365

D38 -1.00301 0.00000 0.00013 -0.00095 -0.00082 -1.00383

D39 1.01965 0.00000 0.00013 -0.00092 -0.00079 1.01886

D40 1.02485 0.00000 0.00022 -0.00106 -0.00083 1.02401

D41 -3.12846 -0.00001 0.00015 -0.00105 -0.00090 -3.12935

D42 -1.10579 -0.00001 0.00014 -0.00101 -0.00087 -1.10666

D43 -1.00449 0.00000 0.00019 -0.00100 -0.00081 -1.00530

D44 1.12539 -0.00001 0.00011 -0.00099 -0.00087 1.12452

D45 -3.13513 -0.00001 0.00011 -0.00095 -0.00084 -3.13598

D46 3.13786 0.00000 -0.00013 -0.00047 -0.00061 3.13725

D47 -1.04995 -0.00001 -0.00015 -0.00045 -0.00060 -1.05055

D48 1.04208 -0.00001 -0.00013 -0.00057 -0.00069 1.04139

D49 1.01165 0.00000 -0.00005 -0.00048 -0.00054 1.01111

D50 3.10703 0.00000 -0.00007 -0.00046 -0.00053 3.10649

D51 -1.08413 0.00000 -0.00005 -0.00058 -0.00062 -1.08475

D52 -1.01750 0.00000 -0.00007 -0.00051 -0.00058 -1.01807

D53 1.07788 0.00000 -0.00009 -0.00049 -0.00057 1.07731

D54 -3.11327 0.00000 -0.00006 -0.00060 -0.00066 -3.11394

Item Value Threshold Converged?

Maximum Force 0.000059 0.000450 YES

RMS Force 0.000014 0.000300 YES

Maximum Displacement 0.015052 0.001800 NO

RMS Displacement 0.002687 0.001200 NO

Predicted change in Energy=-1.661954D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 18:00:37 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.097332 -0.406717 -0.194197

2 6 0 -2.843270 0.074300 0.474804

3 8 0 -4.912164 0.311533 -0.730719

4 8 0 -4.224375 -1.751867 -0.185099

5 6 0 -2.291018 -0.813859 1.572733

6 16 0 -1.583791 0.300286 -0.944640

7 6 0 -0.119029 0.773230 -0.103054

8 16 0 1.079475 -0.555805 0.007070

9 16 0 0.022060 2.254421 0.763368

10 6 0 2.685633 0.336208 -0.009264

11 6 0 3.842301 -0.655386 -0.072036

12 6 0 5.201357 0.050630 -0.064643

13 6 0 6.372217 -0.927379 -0.138270

14 1 0 -3.037620 1.080907 0.842097

15 1 0 -5.039157 -1.968842 -0.668673

16 1 0 -1.384594 -0.367287 1.983560

17 1 0 -3.017377 -0.910250 2.386063

18 1 0 -2.049899 -1.811374 1.205089

19 1 0 2.688680 0.999511 -0.877233

20 1 0 2.745842 0.952127 0.888191

21 1 0 3.787592 -1.343499 0.779972

22 1 0 3.757229 -1.269740 -0.975720

23 1 0 5.250720 0.747734 -0.909481

24 1 0 5.288154 0.660448 0.842323

25 1 0 7.332642 -0.403216 -0.136203

26 1 0 6.369584 -1.615125 0.713809

27 1 0 6.328302 -1.532626 -1.049623

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.500536 0.000000

3 O 1.211483 2.406219 0.000000

4 O 1.351167 2.382815 2.242403 0.000000

5 C 2.559409 1.516330 3.666443 2.776275 0.000000

6 S 2.716782 1.911068 3.335260 3.429419 2.842298

7 C 4.150600 2.871222 4.856056 4.820448 3.169331

8 S 5.182862 4.000467 6.098881 5.440434 3.725335

9 S 4.996796 3.611968 5.509417 5.914570 3.926799

10 C 6.826034 5.556229 7.632013 7.220746 5.347188

11 C 7.944466 6.747470 8.832297 8.141641 6.352007

12 C 9.310830 8.062729 10.138789 9.597288 7.717773

13 C 10.482636 9.290017 11.367636 10.628722 8.831311

14 H 2.099980 1.089006 2.565074 3.238538 2.163650

15 H 1.884781 3.209967 2.284751 0.972004 3.729632

16 H 3.478955 2.144546 4.502428 3.832036 1.090784

17 H 2.842110 2.156979 3.846726 2.962438 1.094712

18 H 2.850095 2.172215 4.055447 2.581572 1.090108

19 H 6.963760 5.769445 7.633322 7.472580 5.838496

20 H 7.060244 5.672711 7.853426 7.552977 5.381196

21 H 7.999911 6.787607 8.983712 8.080207 6.152925

22 H 7.940384 6.890359 8.815828 8.035143 6.579037

23 H 9.446187 8.239080 10.173812 9.825994 8.091834

24 H 9.502660 8.160803 10.326795 9.867273 7.755703

25 H 11.430121 10.205418 12.280049 11.635545 9.782839

26 H 10.575492 9.369523 11.535879 10.632906 8.739897

27 H 10.521086 9.435244 11.395205 10.590300 9.038034

6 7 8 9 10

6 S 0.000000

7 C 1.754272 0.000000

8 S 2.954933 1.793007 0.000000

9 S 3.051998 1.721778 3.096367 0.000000

10 C 4.370834 2.840055 1.837306 3.372110 0.000000

11 C 5.578281 4.211181 2.765752 4.874333 1.524822

12 C 6.846529 5.369370 4.166871 5.689237 2.532487

13 C 8.090454 6.710408 5.307759 7.159700 3.899256

14 H 2.432163 3.083205 4.508499 3.277953 5.833953

15 H 4.143025 5.660967 6.315929 6.745562 8.088291

16 H 3.009932 2.693770 3.164442 3.215727 4.586175

17 H 3.822846 4.174954 4.750731 4.678297 6.309958

18 H 3.049212 3.481333 3.578363 4.584629 5.339664

19 H 4.329834 2.921263 2.406353 3.373016 1.092405

20 H 4.746566 3.036784 2.413921 3.021679 1.090141

21 H 5.876058 4.530117 2.924335 5.208122 2.158384

22 H 5.567085 4.467734 2.940399 5.421774 2.159033

23 H 6.849232 5.430025 4.465262 5.692752 2.749439

24 H 7.109611 5.490363 4.459809 5.502612 2.757435

25 H 8.980605 7.544039 6.256669 7.830510 4.707182

26 H 8.347180 6.962298 5.441221 7.434172 4.231079

27 H 8.122302 6.912383 5.442514 7.576104 4.224207

11 12 13 14 15

11 C 0.000000

12 C 1.531517 0.000000

13 C 2.545356 1.527362 0.000000

14 H 7.154276 8.352508 9.671574 0.000000

15 H 8.997858 10.455202 11.471069 3.948360 0.000000

16 H 5.623959 6.909743 8.061264 2.476428 4.791153

17 H 7.291255 8.629997 9.723015 2.519711 3.813085

18 H 6.138842 7.593417 8.574269 3.077766 3.531493

19 H 2.172066 2.806105 4.222252 5.979400 8.280946

20 H 2.169875 2.783908 4.211503 5.785079 8.459438

21 H 1.096544 2.157707 2.774276 7.243281 8.966667

22 H 1.096045 2.158459 2.767073 7.416196 8.829463

23 H 2.157244 1.096423 2.158361 8.477948 10.645155

24 H 2.158230 1.096357 2.158228 8.336384 10.763346

25 H 3.500026 2.180246 1.094152 10.521503 12.481832

26 H 2.815281 2.178412 1.095007 9.786752 11.497640

27 H 2.811659 2.178735 1.094905 9.906041 11.382202

16 17 18 19 20

16 H 0.000000

17 H 1.767144 0.000000

18 H 1.770320 1.772777 0.000000

19 H 5.161767 6.845098 5.889929 0.000000

20 H 4.472270 6.239132 5.544050 1.766984 0.000000

21 H 5.399363 7.005344 5.871620 3.073049 2.523262

22 H 6.000842 7.571401 6.226719 2.510178 3.071443

23 H 7.323958 9.053781 8.019942 2.574584 3.089954

24 H 6.847206 8.592560 7.751678 3.135140 2.559400

25 H 8.971338 10.664981 9.581965 4.907459 4.891326

26 H 7.955919 9.560770 8.436086 4.787148 4.444400

27 H 8.369408 9.976623 8.680765 4.437148 4.771073

21 22 23 24 25

21 H 0.000000

22 H 1.757503 0.000000

23 H 3.060759 2.510996 0.000000

24 H 2.504272 3.061803 1.754376 0.000000

25 H 3.780329 3.773491 2.501409 2.503762 0.000000

26 H 2.597083 3.130207 3.077341 2.522744 1.765991

27 H 3.136622 2.585534 2.526037 3.077489 1.765957

26 27

26 H 0.000000

27 H 1.765843 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.28D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.104514 -0.466378 -0.119722

2 6 0 -2.845665 0.115551 0.453224

3 8 0 -4.923233 0.156043 -0.760021

4 8 0 -4.231439 -1.792017 0.108805

5 6 0 -2.285454 -0.582971 1.676942

6 16 0 -1.596493 0.106384 -0.993036

7 6 0 -0.125700 0.708161 -0.249999

8 16 0 1.073618 -0.586666 0.066122

9 16 0 0.021596 2.310320 0.363117

10 6 0 2.679582 0.289000 -0.106456

11 6 0 3.835804 -0.700927 -0.015476

12 6 0 5.194851 -0.004646 -0.132646

13 6 0 6.365184 -0.982949 -0.054687

14 1 0 -3.037391 1.168692 0.653395

15 1 0 -5.049688 -2.083778 -0.327239

16 1 0 -1.376099 -0.076595 2.003235

17 1 0 -3.005908 -0.545056 2.500290

18 1 0 -2.046962 -1.627251 1.474612

19 1 0 2.676327 0.802402 -1.070695

20 1 0 2.746258 1.042531 0.678499

21 1 0 3.787283 -1.241343 0.937417

22 1 0 3.744220 -1.453896 -0.806654

23 1 0 5.238076 0.545814 -1.079888

24 1 0 5.288183 0.744380 0.662494

25 1 0 7.325580 -0.466514 -0.144706

26 1 0 6.368739 -1.523051 0.897844

27 1 0 6.314702 -1.728226 -0.855206

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3041720 0.1935795 0.1808642

Leave Link 202 at Sat Aug 17 18:00:37 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.3471698502 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0550002683 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.2921695819 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2322

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.61D-08

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 97

GePol: Fraction of low-weight points (<1% of avg) = 4.18%

GePol: Cavity surface area = 309.341 Ang\*\*2

GePol: Cavity volume = 320.461 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057933132 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.2863762687 Hartrees.

Leave Link 301 at Sat Aug 17 18:00:37 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 18:00:37 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 18:00:37 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000406 -0.000046 -0.000031 Ang= -0.05 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 18:00:37 2019, MaxMem= 1342177280 cpu: 2.6

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16175052.

Iteration 1 A\*A^-1 deviation from unit magnitude is 4.11D-15 for 2306.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.16D-15 for 739 104.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.44D-15 for 2306.

Iteration 1 A^-1\*A deviation from orthogonality is 5.21D-10 for 2167 894.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.66D-15 for 381.

Iteration 2 A\*A^-1 deviation from orthogonality is 2.39D-15 for 793 117.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 187.

Iteration 2 A^-1\*A deviation from orthogonality is 4.56D-16 for 246 241.

E= -1658.67698376320

DIIS: error= 3.69D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67698376320 IErMin= 1 ErrMin= 3.69D-04

ErrMax= 3.69D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.01D-04 BMatP= 1.01D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.69D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.428 Goal= None Shift= 0.000

Gap= 0.484 Goal= None Shift= 0.000

RMSDP=2.07D-05 MaxDP=6.62D-04 OVMax= 1.70D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.07D-05 CP: 1.00D+00

E= -1658.67702601695 Delta-E= -0.000042253748 Rises=F Damp=F

DIIS: error= 4.88D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67702601695 IErMin= 2 ErrMin= 4.88D-05

ErrMax= 4.88D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.92D-06 BMatP= 1.01D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.707D-01 0.107D+01

Coeff: -0.707D-01 0.107D+01

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.76D-06 MaxDP=6.34D-05 DE=-4.23D-05 OVMax= 2.58D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.41D-06 CP: 1.00D+00 1.07D+00

E= -1658.67702648009 Delta-E= -0.000000463147 Rises=F Damp=F

DIIS: error= 3.75D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67702648009 IErMin= 3 ErrMin= 3.75D-05

ErrMax= 3.75D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.53D-07 BMatP= 1.92D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.319D-01 0.426D+00 0.606D+00

Coeff: -0.319D-01 0.426D+00 0.606D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.68D-06 MaxDP=8.13D-05 DE=-4.63D-07 OVMax= 1.92D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.42D-06 CP: 1.00D+00 1.08D+00 6.44D-01

E= -1658.67702651643 Delta-E= -0.000000036334 Rises=F Damp=F

DIIS: error= 3.46D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67702651643 IErMin= 4 ErrMin= 3.46D-05

ErrMax= 3.46D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.64D-07 BMatP= 7.53D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.109D-01 0.141D+00 0.447D+00 0.423D+00

Coeff: -0.109D-01 0.141D+00 0.447D+00 0.423D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=8.15D-07 MaxDP=3.92D-05 DE=-3.63D-08 OVMax= 9.47D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.84D-07 CP: 1.00D+00 1.08D+00 8.07D-01 5.40D-01

E= -1658.67702661767 Delta-E= -0.000000101244 Rises=F Damp=F

DIIS: error= 1.43D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67702661767 IErMin= 5 ErrMin= 1.43D-06

ErrMax= 1.43D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.14D-09 BMatP= 5.64D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.312D-03-0.114D-01 0.376D-01 0.689D-01 0.905D+00

Coeff: 0.312D-03-0.114D-01 0.376D-01 0.689D-01 0.905D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.29D-07 MaxDP=5.99D-06 DE=-1.01D-07 OVMax= 1.35D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 9.92D-08 CP: 1.00D+00 1.08D+00 8.33D-01 5.77D-01 9.65D-01

E= -1658.67702661820 Delta-E= -0.000000000522 Rises=F Damp=F

DIIS: error= 4.23D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67702661820 IErMin= 6 ErrMin= 4.23D-07

ErrMax= 4.23D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.21D-10 BMatP= 2.14D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.852D-03-0.152D-01-0.934D-02 0.787D-02 0.451D+00 0.565D+00

Coeff: 0.852D-03-0.152D-01-0.934D-02 0.787D-02 0.451D+00 0.565D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=5.44D-08 MaxDP=2.63D-06 DE=-5.22D-10 OVMax= 6.06D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 3.57D-08 CP: 1.00D+00 1.08D+00 8.34D-01 5.88D-01 1.06D+00

CP: 7.21D-01

E= -1658.67702661837 Delta-E= -0.000000000179 Rises=F Damp=F

DIIS: error= 1.07D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67702661837 IErMin= 7 ErrMin= 1.07D-07

ErrMax= 1.07D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.43D-11 BMatP= 6.21D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.225D-03-0.341D-02-0.629D-02-0.414D-02 0.514D-01 0.189D+00

Coeff-Com: 0.773D+00

Coeff: 0.225D-03-0.341D-02-0.629D-02-0.414D-02 0.514D-01 0.189D+00

Coeff: 0.773D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.12D-08 MaxDP=1.41D-06 DE=-1.79D-10 OVMax= 2.75D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.55D-08 CP: 1.00D+00 1.08D+00 8.36D-01 5.89D-01 1.08D+00

CP: 8.37D-01 9.39D-01

E= -1658.67702661839 Delta-E= -0.000000000013 Rises=F Damp=F

DIIS: error= 6.43D-08 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1658.67702661839 IErMin= 8 ErrMin= 6.43D-08

ErrMax= 6.43D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.39D-11 BMatP= 3.43D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.143D-04 0.659D-03-0.201D-02-0.365D-02-0.453D-01 0.123D-01

Coeff-Com: 0.439D+00 0.599D+00

Coeff: -0.143D-04 0.659D-03-0.201D-02-0.365D-02-0.453D-01 0.123D-01

Coeff: 0.439D+00 0.599D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.14D-08 MaxDP=3.85D-07 DE=-1.32D-11 OVMax= 1.26D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 6.90D-09 CP: 1.00D+00 1.08D+00 8.37D-01 5.91D-01 1.09D+00

CP: 8.71D-01 1.12D+00 7.52D-01

E= -1658.67702661840 Delta-E= -0.000000000011 Rises=F Damp=F

DIIS: error= 3.87D-08 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1658.67702661840 IErMin= 9 ErrMin= 3.87D-08

ErrMax= 3.87D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.30D-12 BMatP= 1.39D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.521D-04 0.109D-02-0.158D-03-0.166D-02-0.394D-01-0.285D-01

Coeff-Com: 0.134D+00 0.374D+00 0.560D+00

Coeff: -0.521D-04 0.109D-02-0.158D-03-0.166D-02-0.394D-01-0.285D-01

Coeff: 0.134D+00 0.374D+00 0.560D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.65D-09 MaxDP=2.02D-07 DE=-1.14D-11 OVMax= 5.08D-07

Error on total polarization charges = 0.04162

SCF Done: E(UB3LYP) = -1658.67702662 A.U. after 9 cycles

NFock= 9 Conv=0.46D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655235180871D+03 PE=-6.147335114768D+03 EE= 1.731136531010D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.64

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 18:00:58 2019, MaxMem= 1342177280 cpu: 239.0

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 336

Leave Link 701 at Sat Aug 17 18:00:59 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 18:00:59 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 18:01:02 2019, MaxMem= 1342177280 cpu: 38.3

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.42431298D+00-2.96289033D+00 6.29964288D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000016326 0.000012698 0.000025812

2 6 0.000000067 -0.000018024 -0.000015236

3 8 -0.000000249 0.000011009 0.000018485

4 8 -0.000004579 0.000023717 -0.000031732

5 6 0.000008370 -0.000016078 -0.000009517

6 16 -0.000023541 0.000030576 0.000050971

7 6 0.000021585 0.000010395 0.000033578

8 16 -0.000012127 0.000002151 -0.000007592

9 16 0.000006091 -0.000016614 0.000074206

10 6 0.000005394 0.000003044 0.000000913

11 6 -0.000008603 0.000006338 -0.000014645

12 6 -0.000001085 0.000008655 0.000015081

13 6 0.000000690 0.000001605 -0.000032297

14 1 0.000024037 -0.000019497 0.000045506

15 1 -0.000001986 0.000020926 -0.000043515

16 1 0.000000844 -0.000047446 -0.000001111

17 1 0.000005809 -0.000057666 -0.000010158

18 1 0.000000546 -0.000025391 -0.000042173

19 1 -0.000009820 0.000028842 0.000035388

20 1 0.000008678 -0.000020486 0.000029196

21 1 0.000005950 -0.000013047 -0.000031057

22 1 -0.000001087 0.000038360 -0.000027254

23 1 -0.000002721 0.000021678 0.000023285

24 1 0.000001117 -0.000017272 0.000016780

25 1 -0.000004596 0.000006112 -0.000014322

26 1 -0.000001777 -0.000008842 -0.000047325

27 1 -0.000000683 0.000034256 -0.000041267

-------------------------------------------------------------------

Cartesian Forces: Max 0.000074206 RMS 0.000023606

Leave Link 716 at Sat Aug 17 18:01:02 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000034023 RMS 0.000007629

Search for a local minimum.

Step number 67 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .76290D-05 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43 45 44 47 46

49 48 51 50 53

54 55 56 52 57

59 60 61 62 63

64 65 66 67

DE= -2.48D-06 DEPred=-1.66D-07 R= 1.49D+01

TightC=F SS= 1.41D+00 RLast= 1.39D-02 DXNew= 1.0812D-01 4.1720D-02

Trust test= 1.49D+01 RLast= 1.39D-02 DXMaxT set to 6.43D-02

ITU= 1 1 -1 1 1 1 -1 1 0 -1 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 1 1 1 1 1 -1 -1 0 -1 -1 -1 0 -1 0 0 -1 -1

ITU= 0 0 -1 0 0 -1 1 -1 1 -1 1 1 -1 1 -1 1 1 -1 0 0

ITU= -1 0 0 -1 -1 0 0

Eigenvalues --- 0.00070 0.00157 0.00231 0.00295 0.00314

Eigenvalues --- 0.00332 0.00507 0.00976 0.01852 0.02027

Eigenvalues --- 0.03136 0.03520 0.03536 0.03856 0.04330

Eigenvalues --- 0.04501 0.04764 0.04807 0.05088 0.05303

Eigenvalues --- 0.05386 0.05471 0.05532 0.05713 0.07494

Eigenvalues --- 0.08180 0.08315 0.10587 0.10999 0.11347

Eigenvalues --- 0.12099 0.13969 0.14914 0.15149 0.15663

Eigenvalues --- 0.15995 0.16149 0.16194 0.17124 0.17617

Eigenvalues --- 0.18128 0.19517 0.20219 0.20847 0.22331

Eigenvalues --- 0.22433 0.23210 0.24323 0.25463 0.26633

Eigenvalues --- 0.27853 0.29076 0.29105 0.29507 0.30567

Eigenvalues --- 0.30871 0.32736 0.33535 0.33816 0.33864

Eigenvalues --- 0.33924 0.33965 0.34030 0.34042 0.34119

Eigenvalues --- 0.34194 0.34237 0.34289 0.34945 0.35255

Eigenvalues --- 0.35803 0.37585 0.48637 0.53140 0.82350

En-DIIS/RFO-DIIS IScMMF= 0 using points: 67 66 65 64 63

RFO step: Lambda=-1.78693862D-08.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 1.38D-05 SmlDif= 1.00D-05

RMS Error= 0.2573569087D-04 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 0.85472 0.02253 0.01389 0.01449 0.09436

Iteration 1 RMS(Cart)= 0.00126492 RMS(Int)= 0.00000046

Iteration 2 RMS(Cart)= 0.00000106 RMS(Int)= 0.00000001

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000001

ITry= 1 IFail=0 DXMaxC= 5.79D-03 DCOld= 1.00D+10 DXMaxT= 6.43D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83560 0.00002 0.00001 0.00003 0.00004 2.83564

R2 2.28937 -0.00001 -0.00002 -0.00001 -0.00003 2.28934

R3 2.55333 -0.00001 0.00000 0.00001 0.00001 2.55334

R4 2.86545 -0.00002 -0.00003 -0.00005 -0.00008 2.86537

R5 3.61140 -0.00003 -0.00010 -0.00004 -0.00014 3.61126

R6 2.05792 -0.00001 0.00001 -0.00003 -0.00003 2.05790

R7 1.83682 0.00001 0.00001 -0.00001 0.00000 1.83682

R8 2.06128 0.00000 0.00000 -0.00003 -0.00003 2.06125

R9 2.06871 0.00000 0.00000 -0.00001 -0.00001 2.06870

R10 2.06001 0.00000 0.00001 0.00000 0.00001 2.06001

R11 3.31509 0.00001 0.00002 0.00001 0.00003 3.31513

R12 3.38829 -0.00001 -0.00002 -0.00006 -0.00008 3.38821

R13 3.25369 0.00000 0.00000 0.00001 0.00001 3.25370

R14 3.47201 0.00000 0.00001 -0.00002 -0.00001 3.47200

R15 2.88150 -0.00001 -0.00001 -0.00003 -0.00004 2.88146

R16 2.06435 0.00000 -0.00001 0.00000 -0.00001 2.06434

R17 2.06007 0.00000 0.00000 0.00001 0.00001 2.06008

R18 2.89415 -0.00001 0.00000 -0.00001 -0.00001 2.89414

R19 2.07217 0.00000 0.00000 0.00000 0.00000 2.07217

R20 2.07122 -0.00001 -0.00001 -0.00001 -0.00002 2.07120

R21 2.88630 0.00000 0.00000 -0.00001 -0.00001 2.88628

R22 2.07194 -0.00001 0.00000 -0.00001 -0.00001 2.07192

R23 2.07181 0.00000 0.00000 0.00000 -0.00001 2.07181

R24 2.06765 0.00000 0.00000 -0.00001 -0.00001 2.06764

R25 2.06926 -0.00001 0.00000 -0.00001 -0.00002 2.06925

R26 2.06907 0.00000 0.00000 -0.00001 -0.00001 2.06906

A1 2.17670 0.00002 -0.00001 0.00005 0.00004 2.17675

A2 1.97655 0.00000 0.00004 -0.00005 -0.00001 1.97654

A3 2.12936 -0.00002 -0.00003 -0.00001 -0.00004 2.12932

A4 2.02577 0.00000 0.00008 -0.00001 0.00006 2.02583

A5 1.83128 0.00001 -0.00005 -0.00005 -0.00010 1.83118

A6 1.87290 0.00001 0.00005 0.00016 0.00021 1.87311

A7 1.94662 -0.00002 -0.00002 -0.00008 -0.00010 1.94652

A8 1.94142 -0.00001 0.00003 -0.00011 -0.00008 1.94134

A9 1.83260 0.00000 -0.00010 0.00010 0.00000 1.83260

A10 1.87308 0.00000 -0.00004 0.00004 0.00000 1.87307

A11 1.91299 0.00000 0.00000 0.00002 0.00002 1.91301

A12 1.92610 0.00000 0.00004 -0.00002 0.00002 1.92612

A13 1.95232 -0.00001 -0.00002 -0.00002 -0.00003 1.95229

A14 1.88346 0.00000 0.00000 0.00002 0.00002 1.88348

A15 1.89425 0.00000 -0.00002 0.00004 0.00002 1.89428

A16 1.89311 0.00000 0.00000 -0.00004 -0.00004 1.89306

A17 1.79860 0.00001 -0.00001 0.00017 0.00016 1.79876

A18 1.96899 0.00000 0.00004 0.00006 0.00010 1.96908

A19 2.14332 0.00001 0.00001 0.00003 0.00004 2.14335

A20 2.15553 -0.00001 0.00000 -0.00008 -0.00009 2.15545

A21 1.79663 -0.00003 -0.00005 -0.00012 -0.00017 1.79646

A22 1.92599 0.00001 0.00005 0.00000 0.00004 1.92603

A23 1.87999 -0.00001 -0.00003 -0.00001 -0.00004 1.87996

A24 1.89153 0.00000 0.00003 0.00000 0.00002 1.89156

A25 1.93910 0.00001 0.00002 0.00009 0.00012 1.93922

A26 1.93843 -0.00001 -0.00004 -0.00008 -0.00012 1.93831

A27 1.88693 0.00000 -0.00003 0.00000 -0.00002 1.88691

A28 1.95321 0.00000 -0.00002 0.00003 0.00001 1.95322

A29 1.91585 0.00000 0.00001 -0.00003 -0.00002 1.91583

A30 1.91726 0.00000 0.00000 0.00002 0.00002 1.91727

A31 1.90690 0.00000 -0.00001 -0.00001 -0.00001 1.90689

A32 1.90843 0.00000 0.00000 -0.00005 -0.00004 1.90838

A33 1.85982 0.00000 0.00002 0.00003 0.00005 1.85986

A34 1.96584 0.00000 0.00002 -0.00005 -0.00002 1.96582

A35 1.90639 0.00000 -0.00001 -0.00003 -0.00005 1.90634

A36 1.90780 0.00000 -0.00001 0.00006 0.00005 1.90785

A37 1.91289 0.00000 -0.00001 -0.00002 -0.00002 1.91287

A38 1.91277 0.00000 0.00001 0.00003 0.00004 1.91281

A39 1.85482 0.00000 -0.00001 0.00001 0.00000 1.85483

A40 1.94556 0.00000 -0.00001 0.00002 0.00001 1.94557

A41 1.94209 -0.00001 0.00000 -0.00004 -0.00003 1.94206

A42 1.94265 0.00000 0.00002 0.00000 0.00002 1.94266

A43 1.87709 0.00000 -0.00002 0.00001 0.00000 1.87708

A44 1.87716 0.00000 0.00000 -0.00001 -0.00002 1.87714

A45 1.87592 0.00000 0.00001 0.00002 0.00003 1.87595

D1 2.68467 0.00001 0.00175 -0.00063 0.00112 2.68578

D2 -1.44144 0.00000 0.00173 -0.00077 0.00096 -1.44049

D3 0.50151 0.00001 0.00161 -0.00061 0.00100 0.50252

D4 -0.49261 0.00000 0.00171 -0.00077 0.00093 -0.49168

D5 1.66446 -0.00001 0.00169 -0.00092 0.00077 1.66523

D6 -2.67577 0.00000 0.00157 -0.00075 0.00082 -2.67495

D7 -3.10091 0.00001 0.00011 0.00034 0.00045 -3.10046

D8 0.00609 0.00000 0.00007 0.00020 0.00027 0.00637

D9 3.14127 0.00000 -0.00022 -0.00007 -0.00029 3.14097

D10 -1.06995 0.00000 -0.00020 -0.00005 -0.00025 -1.07020

D11 1.03940 0.00000 -0.00018 -0.00013 -0.00031 1.03909

D12 1.04542 -0.00001 -0.00019 0.00006 -0.00013 1.04529

D13 3.11739 -0.00001 -0.00016 0.00008 -0.00009 3.11730

D14 -1.05645 -0.00001 -0.00015 0.00000 -0.00015 -1.05659

D15 -0.99420 0.00001 -0.00007 0.00004 -0.00002 -0.99423

D16 1.07777 0.00001 -0.00005 0.00007 0.00002 1.07778

D17 -3.09607 0.00001 -0.00003 -0.00001 -0.00004 -3.09611

D18 -3.08824 0.00001 -0.00010 0.00165 0.00154 -3.08669

D19 -0.88133 0.00001 -0.00006 0.00155 0.00149 -0.87983

D20 1.22330 -0.00001 -0.00009 0.00144 0.00135 1.22465

D21 1.81796 0.00000 0.00043 -0.00041 0.00002 1.81798

D22 -1.14209 0.00000 0.00021 -0.00044 -0.00024 -1.14233

D23 2.59984 -0.00001 -0.00044 -0.00073 -0.00118 2.59867

D24 -0.72476 0.00000 -0.00022 -0.00068 -0.00090 -0.72566

D25 -3.03586 -0.00001 -0.00012 -0.00037 -0.00049 -3.03635

D26 -0.91632 0.00000 -0.00008 -0.00027 -0.00035 -0.91667

D27 1.12127 0.00000 -0.00011 -0.00027 -0.00038 1.12089

D28 -3.12560 0.00000 0.00017 -0.00029 -0.00013 -3.12573

D29 -1.00524 0.00000 0.00015 -0.00030 -0.00015 -1.00539

D30 1.03430 0.00000 0.00018 -0.00027 -0.00010 1.03421

D31 1.07351 0.00000 0.00016 -0.00034 -0.00018 1.07333

D32 -3.08930 0.00000 0.00015 -0.00035 -0.00020 -3.08951

D33 -1.04977 0.00000 0.00017 -0.00032 -0.00015 -1.04991

D34 -1.02752 0.00000 0.00020 -0.00035 -0.00015 -1.02767

D35 1.09285 0.00000 0.00019 -0.00036 -0.00017 1.09268

D36 3.13239 0.00000 0.00022 -0.00033 -0.00012 3.13227

D37 -3.13365 0.00000 0.00015 -0.00005 0.00010 -3.13355

D38 -1.00383 0.00000 0.00015 -0.00012 0.00003 -1.00381

D39 1.01886 0.00000 0.00013 -0.00010 0.00003 1.01889

D40 1.02401 0.00000 0.00015 -0.00002 0.00013 1.02414

D41 -3.12935 0.00000 0.00015 -0.00010 0.00005 -3.12930

D42 -1.10666 0.00000 0.00013 -0.00007 0.00006 -1.10660

D43 -1.00530 0.00000 0.00014 -0.00003 0.00010 -1.00520

D44 1.12452 0.00000 0.00014 -0.00011 0.00003 1.12455

D45 -3.13598 0.00000 0.00011 -0.00008 0.00004 -3.13594

D46 3.13725 0.00000 0.00010 -0.00029 -0.00019 3.13706

D47 -1.05055 0.00000 0.00008 -0.00029 -0.00021 -1.05076

D48 1.04139 0.00000 0.00010 -0.00029 -0.00019 1.04120

D49 1.01111 0.00000 0.00010 -0.00021 -0.00010 1.01100

D50 3.10649 0.00000 0.00008 -0.00020 -0.00012 3.10637

D51 -1.08475 0.00000 0.00010 -0.00020 -0.00010 -1.08485

D52 -1.01807 0.00000 0.00011 -0.00023 -0.00012 -1.01819

D53 1.07731 0.00000 0.00009 -0.00022 -0.00013 1.07718

D54 -3.11394 0.00000 0.00011 -0.00022 -0.00011 -3.11404

Item Value Threshold Converged?

Maximum Force 0.000034 0.000450 YES

RMS Force 0.000008 0.000300 YES

Maximum Displacement 0.005793 0.001800 NO

RMS Displacement 0.001265 0.001200 NO

Predicted change in Energy=-4.084425D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 18:01:02 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.096831 -0.407332 -0.195167

2 6 0 -2.843696 0.074795 0.474812

3 8 0 -4.911442 0.310070 -0.733123

4 8 0 -4.223135 -1.752551 -0.185353

5 6 0 -2.291311 -0.812915 1.572980

6 16 0 -1.583515 0.301871 -0.943737

7 6 0 -0.118887 0.773599 -0.101200

8 16 0 1.079302 -0.555732 0.008092

9 16 0 0.022497 2.254059 0.766434

10 6 0 2.685527 0.336139 -0.008951

11 6 0 3.842121 -0.655506 -0.071780

12 6 0 5.201208 0.050443 -0.065153

13 6 0 6.371963 -0.927663 -0.138994

14 1 0 -3.039026 1.081200 0.842097

15 1 0 -5.037091 -1.970305 -0.669971

16 1 0 -1.385464 -0.365648 1.984280

17 1 0 -3.018006 -0.909945 2.385926

18 1 0 -2.049236 -1.810232 1.205415

19 1 0 2.688281 0.999294 -0.877029

20 1 0 2.746119 0.952228 0.888368

21 1 0 3.787695 -1.343274 0.780523

22 1 0 3.756728 -1.270174 -0.975206

23 1 0 5.250234 0.747233 -0.910261

24 1 0 5.288433 0.660583 0.841551

25 1 0 7.332421 -0.403569 -0.137671

26 1 0 6.369732 -1.615010 0.713397

27 1 0 6.327537 -1.533298 -1.050057

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.500555 0.000000

3 O 1.211468 2.406249 0.000000

4 O 1.351172 2.382828 2.242371 0.000000

5 C 2.559442 1.516289 3.666646 2.776076 0.000000

6 S 2.716631 1.910994 3.334595 3.429780 2.842109

7 C 4.150599 2.871359 4.856210 4.820101 3.168491

8 S 5.182247 4.000663 6.098199 5.439268 3.725057

9 S 4.997653 3.612381 5.511036 5.914746 3.925628

10 C 6.825526 5.556495 7.631451 7.219651 5.347126

11 C 7.943788 6.747758 8.831454 8.140317 6.352086

12 C 9.310209 8.063041 10.138012 9.596014 7.717947

13 C 10.481867 9.290320 11.366627 10.627262 8.831553

14 H 2.100142 1.088992 2.565522 3.238505 2.163548

15 H 1.884784 3.209975 2.284707 0.972005 3.729569

16 H 3.478970 2.144510 4.502599 3.831865 1.090768

17 H 2.842274 2.156956 3.847338 2.962060 1.094706

18 H 2.849983 2.172159 4.055347 2.581356 1.090113

19 H 6.962850 5.769310 7.632269 7.471195 5.838064

20 H 7.060341 5.673354 7.853652 7.552432 5.381462

21 H 7.999607 6.788205 8.983299 8.079222 6.153339

22 H 7.939229 6.890362 8.814361 8.033354 6.578839

23 H 9.445211 8.239072 10.172618 9.824416 8.091690

24 H 9.502547 8.161444 10.326660 9.866493 7.756205

25 H 11.429398 10.205750 12.279090 11.634127 9.783155

26 H 10.575108 9.370145 11.535304 10.631816 8.740475

27 H 10.519795 9.435184 11.393555 10.588317 9.037910

6 7 8 9 10

6 S 0.000000

7 C 1.754289 0.000000

8 S 2.955005 1.792964 0.000000

9 S 3.052048 1.721784 3.096263 0.000000

10 C 4.370323 2.839827 1.837304 3.372146 0.000000

11 C 5.578028 4.211031 2.765773 4.874187 1.524800

12 C 6.845991 5.369139 4.166884 5.689157 2.532475

13 C 8.090055 6.710204 5.307751 7.159530 3.899220

14 H 2.432091 3.084095 4.509516 3.279366 5.835230

15 H 4.143056 5.660498 6.314352 6.745957 8.086746

16 H 3.009665 2.692829 3.164888 3.213778 4.586768

17 H 3.822684 4.174328 4.750525 4.677429 6.310186

18 H 3.049053 3.479895 3.577024 4.582929 5.338499

19 H 4.328867 2.921137 2.406317 3.373694 1.092402

20 H 4.746083 3.036349 2.413941 3.021217 1.090146

21 H 5.876178 4.529897 2.924426 5.207468 2.158349

22 H 5.566912 4.467805 2.940394 5.421993 2.159019

23 H 6.848328 5.429800 4.465173 5.693072 2.749378

24 H 7.109121 5.490051 4.459917 5.502263 2.757487

25 H 8.980050 7.543808 6.256669 7.830415 4.707161

26 H 8.347135 6.962126 5.441340 7.433701 4.231091

27 H 8.121815 6.912198 5.442360 7.576097 4.224090

11 12 13 14 15

11 C 0.000000

12 C 1.531511 0.000000

13 C 2.545327 1.527354 0.000000

14 H 7.155522 8.353862 9.672889 0.000000

15 H 8.995939 10.453324 11.468894 3.948455 0.000000

16 H 5.624859 6.910684 8.062370 2.476332 4.791070

17 H 7.291529 8.630505 9.723531 2.519625 3.813079

18 H 6.137809 7.592456 8.573386 3.077672 3.531285

19 H 2.172127 2.806111 4.222247 5.980313 8.279056

20 H 2.169772 2.783860 4.211437 5.786768 8.458604

21 H 1.096543 2.157692 2.774290 7.244721 8.965152

22 H 1.096033 2.158413 2.766950 7.417131 8.826925

23 H 2.157199 1.096415 2.158333 8.479040 10.642923

24 H 2.158259 1.096354 2.158247 8.338075 10.762096

25 H 3.500002 2.180243 1.094147 10.522899 12.479697

26 H 2.815310 2.178377 1.094998 9.788301 11.495892

27 H 2.811555 2.178736 1.094899 9.906985 11.379376

16 17 18 19 20

16 H 0.000000

17 H 1.767137 0.000000

18 H 1.770324 1.772749 0.000000

19 H 5.161933 6.844982 5.888470 0.000000

20 H 4.473008 6.239833 5.543206 1.766971 0.000000

21 H 5.400588 7.005902 5.870974 3.073079 2.523061

22 H 6.001572 7.571261 6.225431 2.510319 3.071369

23 H 7.324572 9.053998 8.018664 2.574537 3.089932

24 H 6.848349 8.593520 7.751046 3.135129 2.559416

25 H 8.972493 10.665660 9.581131 4.907414 4.891330

26 H 7.957331 9.561595 8.435592 4.787183 4.444311

27 H 8.370244 9.976659 8.679525 4.437132 4.770942

21 22 23 24 25

21 H 0.000000

22 H 1.757523 0.000000

23 H 3.060717 2.510917 0.000000

24 H 2.504273 3.061788 1.754370 0.000000

25 H 3.780372 3.773334 2.501348 2.503834 0.000000

26 H 2.597164 3.130188 3.077293 2.522688 1.765978

27 H 3.136547 2.585322 2.526053 3.077504 1.765936

26 27

26 H 0.000000

27 H 1.765850 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.90D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.104179 -0.467379 -0.120221

2 6 0 -2.846215 0.116559 0.452674

3 8 0 -4.922706 0.153121 -0.762598

4 8 0 -4.230367 -1.792660 0.110805

5 6 0 -2.285825 -0.579844 1.677467

6 16 0 -1.596400 0.106652 -0.992926

7 6 0 -0.125692 0.708362 -0.249626

8 16 0 1.073301 -0.586483 0.067412

9 16 0 0.021957 2.310819 0.362642

10 6 0 2.679332 0.288672 -0.107090

11 6 0 3.835468 -0.701208 -0.014880

12 6 0 5.194546 -0.005295 -0.133790

13 6 0 6.364762 -0.983640 -0.054763

14 1 0 -3.038898 1.169771 0.651471

15 1 0 -5.047822 -2.085934 -0.325718

16 1 0 -1.377022 -0.072279 2.003395

17 1 0 -3.006581 -0.541506 2.500525

18 1 0 -2.046401 -1.624191 1.476568

19 1 0 2.675748 0.800614 -1.072100

20 1 0 2.746435 1.043400 0.676683

21 1 0 3.787268 -1.239954 0.938973

22 1 0 3.743522 -1.455506 -0.804733

23 1 0 5.237398 0.543536 -1.081986

24 1 0 5.288350 0.745071 0.660025

25 1 0 7.325189 -0.467531 -0.146242

26 1 0 6.368757 -1.522019 0.898733

27 1 0 6.313725 -1.730328 -0.853924

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3036114 0.1936044 0.1808858

Leave Link 202 at Sat Aug 17 18:01:03 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.3694109932 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0550026696 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.3144083236 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2317

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.13D-07

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 90

GePol: Fraction of low-weight points (<1% of avg) = 3.88%

GePol: Cavity surface area = 309.328 Ang\*\*2

GePol: Cavity volume = 320.451 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057910913 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.3086172323 Hartrees.

Leave Link 301 at Sat Aug 17 18:01:03 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 18:01:03 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 18:01:03 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000402 0.000006 0.000001 Ang= 0.05 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 18:01:03 2019, MaxMem= 1342177280 cpu: 2.7

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16105467.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.00D-15 for 2305.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.61D-15 for 811 99.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.33D-15 for 2305.

Iteration 1 A^-1\*A deviation from orthogonality is 1.13D-12 for 910 738.

E= -1658.67701811557

DIIS: error= 7.03D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67701811557 IErMin= 1 ErrMin= 7.03D-05

ErrMax= 7.03D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.22D-05 BMatP= 1.22D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 0.428 Goal= None Shift= 0.000

Gap= 0.484 Goal= None Shift= 0.000

RMSDP=7.05D-06 MaxDP=1.87D-04 OVMax= 4.83D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 7.05D-06 CP: 1.00D+00

E= -1658.67702302964 Delta-E= -0.000004914065 Rises=F Damp=F

DIIS: error= 1.17D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67702302964 IErMin= 2 ErrMin= 1.17D-05

ErrMax= 1.17D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.97D-07 BMatP= 1.22D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.637D-01 0.106D+01

Coeff: -0.637D-01 0.106D+01

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.23D-06 MaxDP=3.46D-05 DE=-4.91D-06 OVMax= 7.83D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.12D-06 CP: 1.00D+00 1.07D+00

E= -1658.67702305703 Delta-E= -0.000000027387 Rises=F Damp=F

DIIS: error= 2.03D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67702305703 IErMin= 2 ErrMin= 1.17D-05

ErrMax= 2.03D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.00D-07 BMatP= 1.97D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.410D-01 0.579D+00 0.462D+00

Coeff: -0.410D-01 0.579D+00 0.462D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.92D-07 MaxDP=2.95D-05 DE=-2.74D-08 OVMax= 7.42D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 4.68D-07 CP: 1.00D+00 1.09D+00 5.57D-01

E= -1658.67702308829 Delta-E= -0.000000031265 Rises=F Damp=F

DIIS: error= 8.58D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67702308829 IErMin= 4 ErrMin= 8.58D-06

ErrMax= 8.58D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.50D-08 BMatP= 1.97D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.120D-01 0.160D+00 0.299D+00 0.553D+00

Coeff: -0.120D-01 0.160D+00 0.299D+00 0.553D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.42D-07 MaxDP=8.58D-06 DE=-3.13D-08 OVMax= 2.48D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.64D-07 CP: 1.00D+00 1.10D+00 6.55D-01 7.10D-01

E= -1658.67702309435 Delta-E= -0.000000006059 Rises=F Damp=F

DIIS: error= 1.34D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67702309435 IErMin= 5 ErrMin= 1.34D-06

ErrMax= 1.34D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.11D-09 BMatP= 3.50D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.381D-02 0.464D-01 0.134D+00 0.304D+00 0.520D+00

Coeff: -0.381D-02 0.464D-01 0.134D+00 0.304D+00 0.520D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.70D-08 MaxDP=3.45D-06 DE=-6.06D-09 OVMax= 4.96D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 5.07D-08 CP: 1.00D+00 1.10D+00 6.72D-01 7.67D-01 8.26D-01

E= -1658.67702309476 Delta-E= -0.000000000406 Rises=F Damp=F

DIIS: error= 4.43D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67702309476 IErMin= 6 ErrMin= 4.43D-07

ErrMax= 4.43D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.10D-10 BMatP= 2.11D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.448D-03-0.104D-01 0.101D-01 0.492D-01 0.260D+00 0.690D+00

Coeff: 0.448D-03-0.104D-01 0.101D-01 0.492D-01 0.260D+00 0.690D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=3.04D-08 MaxDP=1.37D-06 DE=-4.06D-10 OVMax= 3.14D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.17D-08 CP: 1.00D+00 1.10D+00 6.86D-01 7.90D-01 8.72D-01

CP: 8.74D-01

E= -1658.67702309480 Delta-E= -0.000000000040 Rises=F Damp=F

DIIS: error= 9.52D-08 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67702309480 IErMin= 7 ErrMin= 9.52D-08

ErrMax= 9.52D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.02D-11 BMatP= 2.10D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.502D-03-0.861D-02-0.493D-02 0.131D-02 0.850D-01 0.329D+00

Coeff-Com: 0.598D+00

Coeff: 0.502D-03-0.861D-02-0.493D-02 0.131D-02 0.850D-01 0.329D+00

Coeff: 0.598D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.23D-08 MaxDP=5.75D-07 DE=-4.05D-11 OVMax= 1.05D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 9.28D-09 CP: 1.00D+00 1.10D+00 6.86D-01 7.96D-01 9.09D-01

CP: 9.46D-01 9.44D-01

E= -1658.67702309479 Delta-E= 0.000000000004 Rises=F Damp=F

DIIS: error= 2.98D-08 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 7 EnMin= -1658.67702309480 IErMin= 8 ErrMin= 2.98D-08

ErrMax= 2.98D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.34D-12 BMatP= 2.02D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.109D-03-0.140D-02-0.331D-02-0.753D-02-0.101D-01 0.124D-01

Coeff-Com: 0.235D+00 0.775D+00

Coeff: 0.109D-03-0.140D-02-0.331D-02-0.753D-02-0.101D-01 0.124D-01

Coeff: 0.235D+00 0.775D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=6.65D-09 MaxDP=3.02D-07 DE= 3.64D-12 OVMax= 1.23D-06

Error on total polarization charges = 0.04162

SCF Done: E(UB3LYP) = -1658.67702309 A.U. after 8 cycles

NFock= 8 Conv=0.67D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655235538350D+03 PE=-6.147379845373D+03 EE= 1.731158666696D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.63

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 18:01:22 2019, MaxMem= 1342177280 cpu: 211.4

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 336

Leave Link 701 at Sat Aug 17 18:01:23 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 18:01:23 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 18:01:26 2019, MaxMem= 1342177280 cpu: 38.3

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.42368159D+00-2.96229844D+00 6.30540870D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000006323 -0.000009492 0.000017513

2 6 0.000003423 -0.000008305 0.000001515

3 8 -0.000010836 0.000037963 0.000019604

4 8 0.000001001 0.000026958 -0.000027948

5 6 -0.000001150 -0.000048351 -0.000001941

6 16 -0.000006404 0.000033977 0.000017061

7 6 0.000006870 0.000008884 0.000027234

8 16 -0.000008265 0.000006487 -0.000007805

9 16 -0.000004049 -0.000016369 0.000073536

10 6 0.000012660 0.000008027 0.000024414

11 6 -0.000001855 0.000007798 -0.000016410

12 6 -0.000004155 0.000010192 0.000003267

13 6 0.000002765 0.000002371 -0.000024393

14 1 -0.000000426 -0.000012655 0.000049079

15 1 -0.000002834 0.000024214 -0.000039503

16 1 0.000005543 -0.000044295 0.000003385

17 1 0.000003495 -0.000056282 -0.000008433

18 1 0.000000907 -0.000025066 -0.000037582

19 1 -0.000002337 0.000025701 0.000031921

20 1 0.000001230 -0.000021002 0.000027036

21 1 0.000002804 -0.000017821 -0.000034897

22 1 -0.000003151 0.000030653 -0.000032074

23 1 -0.000000830 0.000029142 0.000021831

24 1 0.000001734 -0.000019309 0.000019510

25 1 -0.000000165 0.000007589 -0.000011409

26 1 -0.000000023 -0.000017051 -0.000048280

27 1 -0.000002276 0.000036040 -0.000046232

-------------------------------------------------------------------

Cartesian Forces: Max 0.000073536 RMS 0.000023084

Leave Link 716 at Sat Aug 17 18:01:26 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000017938 RMS 0.000004192

Search for a local minimum.

Step number 68 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .41920D-05 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43 45 44 47 46

49 48 51 50 53

54 55 56 52 57

59 60 61 62 63

64 65 66 67 68

DE= 3.52D-06 DEPred=-4.08D-08 R=-8.63D+01

Trust test=-8.63D+01 RLast= 3.97D-03 DXMaxT set to 5.00D-02

ITU= -1 1 1 -1 1 1 1 -1 1 0 -1 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 1 1 1 1 1 -1 -1 0 -1 -1 -1 0 -1 0 0 -1

ITU= -1 0 0 -1 0 0 -1 1 -1 1 -1 1 1 -1 1 -1 1 1 -1 0

ITU= 0 -1 0 0 -1 -1 0 0

Eigenvalues --- 0.00067 0.00182 0.00251 0.00299 0.00310

Eigenvalues --- 0.00347 0.00528 0.01147 0.01886 0.02082

Eigenvalues --- 0.03100 0.03529 0.03698 0.03991 0.04313

Eigenvalues --- 0.04458 0.04804 0.04826 0.05084 0.05214

Eigenvalues --- 0.05402 0.05472 0.05561 0.05710 0.06927

Eigenvalues --- 0.08111 0.08319 0.10480 0.10966 0.11423

Eigenvalues --- 0.12117 0.14175 0.14912 0.15230 0.15523

Eigenvalues --- 0.15838 0.16172 0.16286 0.17096 0.17803

Eigenvalues --- 0.18277 0.19597 0.20254 0.20899 0.22326

Eigenvalues --- 0.22539 0.23184 0.24640 0.25477 0.27414

Eigenvalues --- 0.27838 0.29030 0.29426 0.29601 0.30642

Eigenvalues --- 0.31203 0.33168 0.33614 0.33765 0.33866

Eigenvalues --- 0.33935 0.33959 0.34016 0.34083 0.34137

Eigenvalues --- 0.34162 0.34263 0.34429 0.34925 0.35493

Eigenvalues --- 0.36331 0.37699 0.48505 0.53265 0.82778

En-DIIS/RFO-DIIS IScMMF= 0 using points: 68 67 66 65 64

RFO step: Lambda=-5.90181818D-09.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= -1.45D-05 SmlDif= 1.00D-05

RMS Error= 0.1611889685D-04 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 0.76308 0.16276 0.08239 0.00277 -0.01099

Iteration 1 RMS(Cart)= 0.00059097 RMS(Int)= 0.00000020

Iteration 2 RMS(Cart)= 0.00000023 RMS(Int)= 0.00000000

ITry= 1 IFail=0 DXMaxC= 2.14D-03 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83564 0.00000 0.00000 0.00000 0.00000 2.83563

R2 2.28934 0.00002 0.00001 0.00004 0.00004 2.28939

R3 2.55334 -0.00001 0.00000 -0.00004 -0.00004 2.55330

R4 2.86537 0.00001 0.00001 0.00003 0.00004 2.86541

R5 3.61126 0.00000 0.00005 -0.00012 -0.00007 3.61118

R6 2.05790 0.00001 0.00001 0.00002 0.00003 2.05793

R7 1.83682 0.00000 0.00000 0.00001 0.00001 1.83684

R8 2.06125 0.00000 0.00001 0.00001 0.00002 2.06127

R9 2.06870 0.00000 0.00000 0.00000 0.00000 2.06870

R10 2.06001 0.00000 0.00000 0.00000 0.00000 2.06001

R11 3.31513 0.00000 -0.00001 0.00006 0.00005 3.31518

R12 3.38821 0.00000 0.00001 -0.00002 -0.00001 3.38820

R13 3.25370 0.00000 0.00000 -0.00001 -0.00001 3.25369

R14 3.47200 0.00001 0.00000 0.00008 0.00007 3.47208

R15 2.88146 0.00000 0.00001 -0.00002 -0.00001 2.88145

R16 2.06434 0.00000 0.00001 -0.00001 -0.00001 2.06433

R17 2.06008 0.00000 0.00000 -0.00001 -0.00001 2.06007

R18 2.89414 0.00000 0.00000 0.00000 0.00000 2.89414

R19 2.07217 0.00000 0.00000 0.00000 0.00000 2.07217

R20 2.07120 0.00000 0.00001 -0.00001 0.00000 2.07120

R21 2.88628 0.00000 0.00000 0.00001 0.00001 2.88629

R22 2.07192 0.00000 0.00001 -0.00001 0.00000 2.07192

R23 2.07181 0.00000 0.00000 0.00000 0.00001 2.07182

R24 2.06764 0.00000 0.00001 0.00000 0.00000 2.06764

R25 2.06925 0.00000 0.00001 -0.00001 -0.00001 2.06924

R26 2.06906 0.00000 0.00000 0.00000 0.00001 2.06906

A1 2.17675 0.00000 -0.00003 0.00005 0.00002 2.17676

A2 1.97654 0.00000 0.00002 -0.00003 -0.00001 1.97653

A3 2.12932 0.00000 0.00001 -0.00002 -0.00001 2.12931

A4 2.02583 0.00000 0.00000 0.00001 0.00001 2.02584

A5 1.83118 0.00000 -0.00001 0.00006 0.00005 1.83123

A6 1.87311 0.00000 -0.00005 0.00009 0.00003 1.87314

A7 1.94652 0.00000 0.00005 -0.00003 0.00002 1.94654

A8 1.94134 0.00000 0.00002 -0.00011 -0.00009 1.94125

A9 1.83260 0.00000 -0.00001 -0.00001 -0.00001 1.83259

A10 1.87307 0.00000 -0.00001 0.00003 0.00001 1.87309

A11 1.91301 0.00000 0.00001 -0.00008 -0.00006 1.91294

A12 1.92612 0.00000 -0.00002 0.00004 0.00003 1.92615

A13 1.95229 0.00000 0.00001 -0.00001 0.00000 1.95229

A14 1.88348 0.00000 -0.00001 0.00002 0.00001 1.88349

A15 1.89428 0.00000 0.00000 0.00001 0.00001 1.89429

A16 1.89306 0.00000 0.00000 0.00002 0.00002 1.89309

A17 1.79876 -0.00001 -0.00003 0.00001 -0.00002 1.79874

A18 1.96908 0.00000 0.00000 -0.00006 -0.00005 1.96903

A19 2.14335 -0.00001 -0.00002 -0.00002 -0.00004 2.14331

A20 2.15545 0.00001 0.00000 0.00004 0.00004 2.15549

A21 1.79646 0.00002 0.00003 -0.00003 0.00001 1.79647

A22 1.92603 0.00001 -0.00001 0.00008 0.00007 1.92610

A23 1.87996 0.00000 0.00003 -0.00011 -0.00008 1.87988

A24 1.89156 0.00000 -0.00002 0.00005 0.00002 1.89158

A25 1.93922 -0.00001 -0.00002 -0.00003 -0.00006 1.93916

A26 1.93831 0.00000 0.00002 0.00002 0.00004 1.93835

A27 1.88691 0.00000 0.00001 -0.00001 0.00000 1.88691

A28 1.95322 0.00000 -0.00001 -0.00003 -0.00004 1.95318

A29 1.91583 0.00000 -0.00001 0.00008 0.00007 1.91590

A30 1.91727 0.00000 0.00001 -0.00004 -0.00003 1.91725

A31 1.90689 0.00000 0.00001 -0.00005 -0.00005 1.90684

A32 1.90838 0.00000 0.00001 0.00004 0.00005 1.90843

A33 1.85986 0.00000 -0.00001 0.00000 -0.00001 1.85986

A34 1.96582 0.00000 0.00001 0.00001 0.00002 1.96584

A35 1.90634 0.00000 0.00002 -0.00001 0.00001 1.90636

A36 1.90785 0.00000 -0.00002 -0.00001 -0.00002 1.90782

A37 1.91287 0.00000 0.00001 -0.00005 -0.00004 1.91283

A38 1.91281 0.00000 -0.00002 0.00004 0.00002 1.91284

A39 1.85483 0.00000 0.00000 0.00001 0.00001 1.85483

A40 1.94557 0.00000 0.00000 -0.00002 -0.00002 1.94555

A41 1.94206 0.00000 0.00001 -0.00002 -0.00001 1.94205

A42 1.94266 0.00000 0.00000 0.00000 -0.00001 1.94266

A43 1.87708 0.00000 -0.00001 0.00003 0.00002 1.87711

A44 1.87714 0.00000 0.00000 0.00000 0.00001 1.87715

A45 1.87595 0.00000 -0.00001 0.00001 0.00001 1.87596

D1 2.68578 0.00000 0.00014 -0.00002 0.00012 2.68590

D2 -1.44049 0.00000 0.00019 0.00000 0.00019 -1.44030

D3 0.50252 0.00000 0.00016 0.00005 0.00021 0.50273

D4 -0.49168 0.00000 0.00019 -0.00014 0.00005 -0.49163

D5 1.66523 0.00000 0.00024 -0.00012 0.00012 1.66535

D6 -2.67495 0.00000 0.00021 -0.00006 0.00014 -2.67481

D7 -3.10046 0.00000 -0.00010 0.00021 0.00012 -3.10034

D8 0.00637 0.00000 -0.00005 0.00010 0.00005 0.00642

D9 3.14097 0.00000 -0.00003 0.00018 0.00015 3.14112

D10 -1.07020 0.00000 -0.00004 0.00018 0.00013 -1.07007

D11 1.03909 0.00000 -0.00004 0.00022 0.00018 1.03927

D12 1.04529 0.00000 -0.00005 0.00011 0.00006 1.04535

D13 3.11730 0.00000 -0.00007 0.00011 0.00005 3.11734

D14 -1.05659 0.00000 -0.00006 0.00015 0.00009 -1.05650

D15 -0.99423 0.00000 -0.00009 0.00021 0.00012 -0.99410

D16 1.07778 0.00000 -0.00010 0.00021 0.00011 1.07789

D17 -3.09611 0.00000 -0.00010 0.00025 0.00015 -3.09595

D18 -3.08669 0.00000 -0.00025 0.00013 -0.00012 -3.08681

D19 -0.87983 0.00000 -0.00023 0.00017 -0.00006 -0.87989

D20 1.22465 0.00000 -0.00018 0.00001 -0.00017 1.22448

D21 1.81798 0.00000 0.00009 0.00010 0.00018 1.81816

D22 -1.14233 0.00001 0.00021 0.00028 0.00048 -1.14185

D23 2.59867 0.00001 0.00020 0.00010 0.00029 2.59896

D24 -0.72566 0.00000 0.00007 -0.00009 -0.00002 -0.72569

D25 -3.03635 0.00001 0.00027 0.00010 0.00037 -3.03598

D26 -0.91667 0.00000 0.00025 0.00004 0.00030 -0.91638

D27 1.12089 0.00000 0.00026 0.00000 0.00026 1.12115

D28 -3.12573 0.00000 0.00006 0.00022 0.00028 -3.12545

D29 -1.00539 0.00000 0.00006 0.00018 0.00025 -1.00514

D30 1.03421 0.00000 0.00006 0.00021 0.00026 1.03447

D31 1.07333 0.00000 0.00005 0.00032 0.00037 1.07370

D32 -3.08951 0.00000 0.00005 0.00029 0.00034 -3.08917

D33 -1.04991 0.00000 0.00004 0.00031 0.00035 -1.04956

D34 -1.02767 0.00000 0.00004 0.00034 0.00038 -1.02729

D35 1.09268 0.00000 0.00004 0.00030 0.00035 1.09302

D36 3.13227 0.00000 0.00003 0.00033 0.00036 3.13263

D37 -3.13355 0.00000 0.00000 0.00024 0.00023 -3.13332

D38 -1.00381 0.00000 0.00003 0.00017 0.00020 -1.00360

D39 1.01889 0.00000 0.00003 0.00018 0.00020 1.01909

D40 1.02414 0.00000 0.00000 0.00020 0.00020 1.02434

D41 -3.12930 0.00000 0.00004 0.00013 0.00017 -3.12913

D42 -1.10660 0.00000 0.00004 0.00014 0.00017 -1.10643

D43 -1.00520 0.00000 0.00001 0.00020 0.00020 -1.00499

D44 1.12455 0.00000 0.00004 0.00014 0.00018 1.12472

D45 -3.13594 0.00000 0.00004 0.00014 0.00018 -3.13577

D46 3.13706 0.00000 0.00010 0.00030 0.00040 3.13746

D47 -1.05076 0.00000 0.00010 0.00030 0.00041 -1.05035

D48 1.04120 0.00000 0.00010 0.00030 0.00041 1.04161

D49 1.01100 0.00000 0.00006 0.00033 0.00040 1.01140

D50 3.10637 0.00000 0.00007 0.00034 0.00041 3.10678

D51 -1.08485 0.00000 0.00007 0.00034 0.00041 -1.08444

D52 -1.01819 0.00000 0.00007 0.00033 0.00040 -1.01779

D53 1.07718 0.00000 0.00007 0.00034 0.00041 1.07759

D54 -3.11404 0.00000 0.00007 0.00034 0.00041 -3.11364

Item Value Threshold Converged?

Maximum Force 0.000018 0.000450 YES

RMS Force 0.000004 0.000300 YES

Maximum Displacement 0.002138 0.001800 NO

RMS Displacement 0.000591 0.001200 YES

Predicted change in Energy=-1.589805D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 18:01:26 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.096935 -0.407372 -0.195158

2 6 0 -2.843703 0.074816 0.474591

3 8 0 -4.911410 0.309935 -0.733499

4 8 0 -4.223478 -1.752543 -0.184737

5 6 0 -2.291418 -0.812549 1.573116

6 16 0 -1.583521 0.301258 -0.944007

7 6 0 -0.118874 0.773273 -0.101607

8 16 0 1.079316 -0.556027 0.007943

9 16 0 0.022245 2.253773 0.765995

10 6 0 2.685567 0.335885 -0.008841

11 6 0 3.842235 -0.655647 -0.071961

12 6 0 5.201249 0.050444 -0.064723

13 6 0 6.372139 -0.927464 -0.139170

14 1 0 -3.038853 1.081381 0.841578

15 1 0 -5.037424 -1.970389 -0.669341

16 1 0 -1.385567 -0.365127 1.984265

17 1 0 -3.018139 -0.909261 2.386079

18 1 0 -2.049348 -1.809997 1.205904

19 1 0 2.688265 0.999207 -0.876788

20 1 0 2.746126 0.951803 0.888592

21 1 0 3.787783 -1.343864 0.779977

22 1 0 3.757014 -1.269860 -0.975715

23 1 0 5.250289 0.747823 -0.909342

24 1 0 5.288302 0.659962 0.842419

25 1 0 7.332531 -0.403250 -0.136990

26 1 0 6.369686 -1.615681 0.712515

27 1 0 6.328083 -1.532167 -1.050873

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.500553 0.000000

3 O 1.211491 2.406278 0.000000

4 O 1.351150 2.382799 2.242366 0.000000

5 C 2.559463 1.516308 3.666715 2.776056 0.000000

6 S 2.716649 1.910957 3.334552 3.429863 2.842111

7 C 4.150619 2.871330 4.856168 4.820210 3.168513

8 S 5.182366 4.000725 6.098231 5.439522 3.725240

9 S 4.997314 3.611984 5.510711 5.914442 3.925151

10 C 6.825648 5.556499 7.631504 7.219929 5.347136

11 C 7.944007 6.747893 8.831551 8.140739 6.352370

12 C 9.310361 8.063045 10.138070 9.596387 7.717987

13 C 10.482134 9.290479 11.366743 10.627790 8.831893

14 H 2.100177 1.089007 2.565632 3.238485 2.163510

15 H 1.884779 3.209962 2.284704 0.972011 3.729578

16 H 3.478963 2.144488 4.502613 3.831870 1.090778

17 H 2.842266 2.156993 3.847425 2.961935 1.094708

18 H 2.850078 2.172174 4.055465 2.581477 1.090112

19 H 6.962903 5.769176 7.632214 7.471496 5.837956

20 H 7.060408 5.673332 7.853727 7.552543 5.381297

21 H 7.999793 6.788411 8.983408 8.079480 6.153702

22 H 7.939627 6.890646 8.814533 8.034108 6.579453

23 H 9.445376 8.238987 10.172649 9.824924 8.091643

24 H 9.502549 8.161323 10.326672 9.866569 7.755924

25 H 11.429615 10.205798 12.279192 11.634613 9.783271

26 H 10.575161 9.370214 11.535253 10.631976 8.740730

27 H 10.520380 9.435628 11.393869 10.589343 9.038748

6 7 8 9 10

6 S 0.000000

7 C 1.754316 0.000000

8 S 2.954970 1.792958 0.000000

9 S 3.052033 1.721780 3.096291 0.000000

10 C 4.370451 2.839860 1.837343 3.372232 0.000000

11 C 5.578079 4.211067 2.765869 4.874343 1.524795

12 C 6.846105 5.369130 4.166943 5.689186 2.532440

13 C 8.090120 6.710229 5.307879 7.159661 3.899211

14 H 2.432056 3.083958 4.509475 3.278801 5.835063

15 H 4.143099 5.660577 6.314558 6.745664 8.087011

16 H 3.009657 2.692829 3.165113 3.213216 4.586723

17 H 3.822690 4.174354 4.750730 4.676899 6.310173

18 H 3.049018 3.479885 3.577162 4.582494 5.338524

19 H 4.328950 2.920956 2.406287 3.373475 1.092398

20 H 4.746312 3.036544 2.413990 3.021537 1.090142

21 H 5.876177 4.530059 2.924469 5.207923 2.158395

22 H 5.566932 4.467770 2.940614 5.421996 2.158995

23 H 6.848472 5.429640 4.465249 5.692722 2.749253

24 H 7.109286 5.490135 4.459882 5.502493 2.757517

25 H 8.980178 7.543799 6.256760 7.830418 4.707125

26 H 8.346988 6.962134 5.441259 7.434080 4.231039

27 H 8.121966 6.912266 5.442747 7.576143 4.224141

11 12 13 14 15

11 C 0.000000

12 C 1.531513 0.000000

13 C 2.545351 1.527360 0.000000

14 H 7.155501 8.353651 9.672853 0.000000

15 H 8.996319 10.453695 11.469390 3.948476 0.000000

16 H 5.625156 6.910658 8.062704 2.476181 4.791091

17 H 7.291845 8.630515 9.723915 2.519636 3.813017

18 H 6.138096 7.592555 8.573770 3.077649 3.531412

19 H 2.172080 2.806187 4.222211 5.979917 8.279360

20 H 2.169795 2.783682 4.211401 5.786621 8.458724

21 H 1.096543 2.157660 2.774367 7.244899 8.965341

22 H 1.096034 2.158453 2.766933 7.417189 8.827613

23 H 2.157208 1.096413 2.158309 8.478611 10.643463

24 H 2.158246 1.096357 2.158272 8.337811 10.762193

25 H 3.500014 2.180235 1.094148 10.522705 12.480189

26 H 2.815150 2.178374 1.094996 9.788329 11.495977

27 H 2.811760 2.178739 1.094902 9.907143 11.380349

16 17 18 19 20

16 H 0.000000

17 H 1.767152 0.000000

18 H 1.770339 1.772764 0.000000

19 H 5.161700 6.844822 5.888481 0.000000

20 H 4.472772 6.239613 5.542996 1.766964 0.000000

21 H 5.401091 7.006355 5.871184 3.073075 2.523278

22 H 6.002180 7.571947 6.226159 2.510114 3.071371

23 H 7.324357 9.053873 8.018816 2.574532 3.089499

24 H 6.848003 8.593154 7.750738 3.135435 2.559289

25 H 8.972537 10.665753 9.581334 4.907484 4.891124

26 H 7.957712 9.561960 8.435717 4.787105 4.444452

27 H 8.371048 9.977600 8.680529 4.436939 4.770958

21 22 23 24 25

21 H 0.000000

22 H 1.757520 0.000000

23 H 3.060698 2.511039 0.000000

24 H 2.504151 3.061808 1.754375 0.000000

25 H 3.780320 3.773433 2.501446 2.503705 0.000000

26 H 2.597047 3.129818 3.077274 2.522859 1.765990

27 H 3.136972 2.585507 2.525871 3.077520 1.765943

26 27

26 H 0.000000

27 H 1.765854 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 9.84D-05

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.104244 -0.467221 -0.120176

2 6 0 -2.846184 0.116694 0.452526

3 8 0 -4.922633 0.153170 -0.762877

4 8 0 -4.230673 -1.792369 0.111350

5 6 0 -2.285898 -0.579397 1.677568

6 16 0 -1.596364 0.106249 -0.993017

7 6 0 -0.125639 0.708162 -0.249851

8 16 0 1.073352 -0.586637 0.067349

9 16 0 0.021751 2.310610 0.362492

10 6 0 2.679415 0.288606 -0.106839

11 6 0 3.835619 -0.701221 -0.015000

12 6 0 5.194631 -0.005067 -0.133278

13 6 0 6.364974 -0.983326 -0.054946

14 1 0 -3.038685 1.170002 0.651074

15 1 0 -5.048118 -2.085699 -0.325167

16 1 0 -1.377091 -0.071731 2.003361

17 1 0 -3.006681 -0.540796 2.500591

18 1 0 -2.046480 -1.623803 1.476969

19 1 0 2.675780 0.800800 -1.071711

20 1 0 2.746486 1.043129 0.677129

21 1 0 3.787385 -1.240537 0.938530

22 1 0 3.743840 -1.455069 -0.805304

23 1 0 5.237506 0.544492 -1.081049

24 1 0 5.288266 0.744703 0.661125

25 1 0 7.325343 -0.466955 -0.145559

26 1 0 6.368735 -1.522743 0.897960

27 1 0 6.314301 -1.729143 -0.854946

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3037965 0.1935949 0.1808827

Leave Link 202 at Sat Aug 17 18:01:26 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 313 symmetry adapted cartesian basis functions of A symmetry.

There are 300 symmetry adapted basis functions of A symmetry.

300 basis functions, 528 primitive gaussians, 313 cartesian basis functions

64 alpha electrons 63 beta electrons

nuclear repulsion energy 1102.3676320929 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 27 NActive= 27 NUniq= 27 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.0550030288 Hartrees.

Nuclear repulsion after empirical dispersion term = 1102.3126290642 Hartrees.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 27.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 27

GePol: Total number of spheres = 27

GePol: Number of exposed spheres = 26 ( 96.30%)

GePol: Number of points = 2318

GePol: Average weight of points = 0.13

GePol: Minimum weight of points = 0.34D-09

GePol: Maximum weight of points = 0.19854

GePol: Number of points with low weight = 90

GePol: Fraction of low-weight points (<1% of avg) = 3.88%

GePol: Cavity surface area = 309.320 Ang\*\*2

GePol: Cavity volume = 320.448 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0057908875 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 1102.3068381766 Hartrees.

Leave Link 301 at Sat Aug 17 18:01:26 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 300 RedAO= T EigKep= 1.85D-03 NBF= 300

NBsUse= 300 1.00D-06 EigRej= -1.00D+00 NBFU= 300

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 295 295 295 295 295 MxSgAt= 27 MxSgA2= 27.

Leave Link 302 at Sat Aug 17 18:01:26 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 18:01:26 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "BTPAanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000042 0.000003 -0.000003 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

Leave Link 401 at Sat Aug 17 18:01:27 2019, MaxMem= 1342177280 cpu: 2.7

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 318573 IEndB= 318573 NGot= 1342177280 MDV= 1341973630

LenX= 1341973630 LenY= 1341875220

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 730000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 16119372.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.22D-15 for 2315.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.69D-15 for 761 627.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.77D-15 for 2315.

Iteration 1 A^-1\*A deviation from orthogonality is 4.27D-08 for 2110 893.

Iteration 2 A\*A^-1 deviation from unit magnitude is 3.33D-15 for 1743.

Iteration 2 A\*A^-1 deviation from orthogonality is 2.59D-15 for 695 430.

Iteration 2 A^-1\*A deviation from unit magnitude is 9.99D-16 for 155.

Iteration 2 A^-1\*A deviation from orthogonality is 3.13D-16 for 186 173.

E= -1658.67702244929

DIIS: error= 4.49D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1658.67702244929 IErMin= 1 ErrMin= 4.49D-05

ErrMax= 4.49D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.77D-06 BMatP= 1.77D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 0.428 Goal= None Shift= 0.000

Gap= 0.484 Goal= None Shift= 0.000

RMSDP=2.51D-06 MaxDP=6.02D-05 OVMax= 2.09D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.51D-06 CP: 1.00D+00

E= -1658.67702328115 Delta-E= -0.000000831862 Rises=F Damp=F

DIIS: error= 3.77D-06 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1658.67702328115 IErMin= 2 ErrMin= 3.77D-06

ErrMax= 3.77D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.12D-08 BMatP= 1.77D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.732D-01 0.107D+01

Coeff: -0.732D-01 0.107D+01

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.58D-07 MaxDP=1.57D-05 DE=-8.32D-07 OVMax= 2.66D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.76D-07 CP: 1.00D+00 1.10D+00

E= -1658.67702329033 Delta-E= -0.000000009173 Rises=F Damp=F

DIIS: error= 1.53D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1658.67702329033 IErMin= 3 ErrMin= 1.53D-06

ErrMax= 1.53D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.18D-09 BMatP= 2.12D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.306D-01 0.390D+00 0.641D+00

Coeff: -0.306D-01 0.390D+00 0.641D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.93D-07 MaxDP=8.13D-06 DE=-9.17D-09 OVMax= 1.12D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.54D-07 CP: 1.00D+00 1.12D+00 7.17D-01

E= -1658.67702329103 Delta-E= -0.000000000700 Rises=F Damp=F

DIIS: error= 1.71D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1658.67702329103 IErMin= 3 ErrMin= 1.53D-06

ErrMax= 1.71D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.49D-09 BMatP= 5.18D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.105D-01 0.121D+00 0.412D+00 0.477D+00

Coeff: -0.105D-01 0.121D+00 0.412D+00 0.477D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=7.52D-08 MaxDP=3.43D-06 DE=-7.00D-10 OVMax= 6.28D-06

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.80D-08 CP: 1.00D+00 1.13D+00 8.09D-01 7.01D-01

E= -1658.67702329149 Delta-E= -0.000000000468 Rises=F Damp=F

DIIS: error= 5.76D-07 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1658.67702329149 IErMin= 5 ErrMin= 5.76D-07

ErrMax= 5.76D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.02D-10 BMatP= 2.49D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.239D-02 0.214D-01 0.160D+00 0.273D+00 0.548D+00

Coeff: -0.239D-02 0.214D-01 0.160D+00 0.273D+00 0.548D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=2.51D-08 MaxDP=7.38D-07 DE=-4.68D-10 OVMax= 1.88D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.85D-08 CP: 1.00D+00 1.13D+00 8.43D-01 7.26D-01 7.87D-01

E= -1658.67702329156 Delta-E= -0.000000000070 Rises=F Damp=F

DIIS: error= 1.79D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1658.67702329156 IErMin= 6 ErrMin= 1.79D-07

ErrMax= 1.79D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.75D-11 BMatP= 2.02D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.546D-03-0.106D-01 0.177D-01 0.729D-01 0.304D+00 0.615D+00

Coeff: 0.546D-03-0.106D-01 0.177D-01 0.729D-01 0.304D+00 0.615D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=1.09D-08 MaxDP=3.80D-07 DE=-7.00D-11 OVMax= 1.01D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 8.69D-09 CP: 1.00D+00 1.13D+00 8.50D-01 7.55D-01 8.43D-01

CP: 8.77D-01

E= -1658.67702329158 Delta-E= -0.000000000015 Rises=F Damp=F

DIIS: error= 5.01D-08 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1658.67702329158 IErMin= 7 ErrMin= 5.01D-08

ErrMax= 5.01D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.38D-12 BMatP= 2.75D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.462D-03-0.655D-02-0.970D-02 0.171D-02 0.634D-01 0.263D+00

Coeff-Com: 0.688D+00

Coeff: 0.462D-03-0.655D-02-0.970D-02 0.171D-02 0.634D-01 0.263D+00

Coeff: 0.688D+00

Gap= 0.121 Goal= None Shift= 0.000

Gap= 0.133 Goal= None Shift= 0.000

RMSDP=4.47D-09 MaxDP=2.64D-07 DE=-1.55D-11 OVMax= 6.21D-07

Error on total polarization charges = 0.04162

SCF Done: E(UB3LYP) = -1658.67702329 A.U. after 7 cycles

NFock= 7 Conv=0.45D-08 -V/T= 2.0021

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7552 S= 0.5026

<L.S>= 0.000000000000E+00

KE= 1.655235388723D+03 PE=-6.147376172389D+03 EE= 1.731156922198D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.63

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7552, after 0.7500

Leave Link 502 at Sat Aug 17 18:01:44 2019, MaxMem= 1342177280 cpu: 196.2

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 336

Leave Link 701 at Sat Aug 17 18:01:45 2019, MaxMem= 1342177280 cpu: 10.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 18:01:45 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Sat Aug 17 18:01:48 2019, MaxMem= 1342177280 cpu: 38.5

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.42386896D+00-2.96174756D+00 6.31112938D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000008108 0.000015884 -0.000007905

2 6 0.000000871 0.000001332 0.000024687

3 8 0.000011359 0.000022011 0.000037657

4 8 -0.000004154 0.000012277 -0.000029420

5 6 0.000005595 -0.000042333 -0.000010800

6 16 -0.000003806 0.000035012 0.000015939

7 6 -0.000002381 0.000006289 0.000029024

8 16 0.000007292 0.000005622 -0.000004010

9 16 0.000002172 -0.000013365 0.000071305

10 6 -0.000001493 0.000006863 0.000014092

11 6 -0.000002143 0.000004268 -0.000014777

12 6 -0.000000534 0.000008667 -0.000000847

13 6 -0.000001669 0.000006597 -0.000026836

14 1 -0.000002567 -0.000019864 0.000041188

15 1 -0.000000033 0.000026785 -0.000035550

16 1 0.000000465 -0.000050426 0.000003348

17 1 0.000003990 -0.000055502 -0.000010948

18 1 -0.000000023 -0.000026469 -0.000035484

19 1 -0.000001401 0.000029913 0.000032615

20 1 0.000000258 -0.000022025 0.000030973

21 1 -0.000001890 -0.000016473 -0.000033067

22 1 -0.000000445 0.000031746 -0.000031209

23 1 -0.000002308 0.000031376 0.000021482

24 1 0.000002592 -0.000021714 0.000017409

25 1 -0.000001030 0.000006568 -0.000012717

26 1 0.000002735 -0.000016741 -0.000044592

27 1 -0.000003344 0.000033703 -0.000041557

-------------------------------------------------------------------

Cartesian Forces: Max 0.000071305 RMS 0.000022562

Leave Link 716 at Sat Aug 17 18:01:48 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000016848 RMS 0.000002547

Search for a local minimum.

Step number 69 out of a maximum of 135

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .25470D-05 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 4 5 6 2

8 9 10 11 12

13 14 15 16 17

18 20 21 22 23

24 19 26 30 31

27 34 35 33 37

38 39 40 41 42

43 45 44 47 46

49 48 51 50 53

54 55 56 52 57

59 60 61 62 63

64 65 66 67 68

69

DE= -1.97D-07 DEPred=-1.59D-08 R= 1.24D+01

Trust test= 1.24D+01 RLast= 1.96D-03 DXMaxT set to 5.00D-02

ITU= 0 -1 1 1 -1 1 1 1 -1 1 0 -1 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 1 1 1 1 1 -1 -1 0 -1 -1 -1 0 -1 0 0

ITU= -1 -1 0 0 -1 0 0 -1 1 -1 1 -1 1 1 -1 1 -1 1 1 -1

ITU= 0 0 -1 0 0 -1 -1 0 0

Eigenvalues --- 0.00069 0.00179 0.00250 0.00306 0.00343

Eigenvalues --- 0.00352 0.00523 0.01038 0.01907 0.02299

Eigenvalues --- 0.03092 0.03527 0.03613 0.03897 0.04328

Eigenvalues --- 0.04620 0.04804 0.04856 0.05125 0.05293

Eigenvalues --- 0.05436 0.05484 0.05531 0.05710 0.07520

Eigenvalues --- 0.08143 0.08327 0.10614 0.11013 0.11696

Eigenvalues --- 0.12115 0.14148 0.14775 0.15214 0.15630

Eigenvalues --- 0.16032 0.16190 0.16301 0.17089 0.17873

Eigenvalues --- 0.18242 0.19850 0.20220 0.21205 0.22416

Eigenvalues --- 0.22560 0.23209 0.24495 0.25645 0.27009

Eigenvalues --- 0.27845 0.28953 0.29420 0.29590 0.30587

Eigenvalues --- 0.30955 0.32754 0.33540 0.33816 0.33867

Eigenvalues --- 0.33926 0.33962 0.34000 0.34065 0.34128

Eigenvalues --- 0.34216 0.34330 0.34394 0.35068 0.35297

Eigenvalues --- 0.36168 0.37118 0.48008 0.53276 0.84405

En-DIIS/RFO-DIIS IScMMF= 0 using points: 69 68 67 66 65

RFO step: Lambda=-1.63522713D-09.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 2.96D-06 SmlDif= 1.00D-05

RMS Error= 0.7274454728D-05 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 0.71269 0.10096 0.13191 0.04978 0.00466

Iteration 1 RMS(Cart)= 0.00031533 RMS(Int)= 0.00000003

Iteration 2 RMS(Cart)= 0.00000006 RMS(Int)= 0.00000000

ITry= 1 IFail=0 DXMaxC= 1.20D-03 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.83563 0.00000 0.00000 0.00000 0.00000 2.83563

R2 2.28939 -0.00002 -0.00001 -0.00001 -0.00002 2.28937

R3 2.55330 0.00000 0.00002 -0.00002 0.00000 2.55330

R4 2.86541 0.00000 0.00000 0.00000 -0.00001 2.86540

R5 3.61118 0.00000 0.00004 -0.00003 0.00001 3.61120

R6 2.05793 0.00000 0.00000 -0.00001 -0.00001 2.05792

R7 1.83684 0.00000 0.00000 0.00000 0.00000 1.83683

R8 2.06127 0.00000 0.00000 0.00000 0.00000 2.06127

R9 2.06870 0.00000 0.00000 0.00000 0.00000 2.06870

R10 2.06001 0.00000 0.00000 0.00000 0.00000 2.06001

R11 3.31518 0.00000 -0.00002 0.00002 0.00000 3.31517

R12 3.38820 0.00000 0.00002 0.00000 0.00002 3.38822

R13 3.25369 0.00000 0.00000 0.00001 0.00001 3.25370

R14 3.47208 0.00000 -0.00002 -0.00001 -0.00003 3.47204

R15 2.88145 0.00000 0.00001 -0.00001 0.00000 2.88145

R16 2.06433 0.00000 0.00000 0.00000 0.00000 2.06434

R17 2.06007 0.00000 0.00000 -0.00001 -0.00001 2.06006

R18 2.89414 0.00000 0.00000 0.00000 0.00000 2.89414

R19 2.07217 0.00000 0.00000 0.00000 0.00000 2.07217

R20 2.07120 0.00000 0.00000 0.00000 0.00000 2.07120

R21 2.88629 0.00000 0.00000 0.00000 0.00000 2.88629

R22 2.07192 0.00000 0.00000 0.00000 0.00000 2.07192

R23 2.07182 0.00000 0.00000 -0.00001 -0.00001 2.07181

R24 2.06764 0.00000 0.00000 0.00000 0.00000 2.06764

R25 2.06924 0.00000 0.00001 0.00000 0.00000 2.06925

R26 2.06906 0.00000 0.00000 0.00000 0.00000 2.06906

A1 2.17676 -0.00001 -0.00002 -0.00001 -0.00003 2.17673

A2 1.97653 0.00000 0.00001 0.00001 0.00003 1.97656

A3 2.12931 0.00000 0.00001 0.00000 0.00001 2.12932

A4 2.02584 0.00000 0.00000 0.00001 0.00001 2.02585

A5 1.83123 0.00000 -0.00001 0.00002 0.00000 1.83123

A6 1.87314 0.00000 -0.00005 0.00001 -0.00004 1.87310

A7 1.94654 0.00000 0.00002 0.00000 0.00002 1.94656

A8 1.94125 0.00000 0.00005 -0.00001 0.00003 1.94128

A9 1.83259 0.00000 -0.00001 -0.00002 -0.00003 1.83256

A10 1.87309 0.00000 -0.00001 0.00000 -0.00002 1.87307

A11 1.91294 0.00000 0.00003 -0.00001 0.00002 1.91297

A12 1.92615 0.00000 -0.00002 -0.00001 -0.00002 1.92613

A13 1.95229 0.00000 0.00000 0.00001 0.00001 1.95230

A14 1.88349 0.00000 -0.00001 -0.00002 -0.00003 1.88346

A15 1.89429 0.00000 -0.00001 0.00001 0.00000 1.89429

A16 1.89309 0.00000 0.00000 0.00001 0.00001 1.89310

A17 1.79874 0.00000 -0.00003 0.00000 -0.00003 1.79871

A18 1.96903 0.00001 0.00002 0.00001 0.00003 1.96906

A19 2.14331 0.00000 0.00000 -0.00001 -0.00002 2.14330

A20 2.15549 0.00000 -0.00001 -0.00001 -0.00002 2.15547

A21 1.79647 0.00000 0.00002 -0.00001 0.00001 1.79648

A22 1.92610 0.00000 -0.00003 0.00001 -0.00002 1.92608

A23 1.87988 0.00000 0.00004 -0.00002 0.00002 1.87989

A24 1.89158 0.00000 -0.00001 -0.00001 -0.00002 1.89156

A25 1.93916 0.00000 0.00000 0.00002 0.00002 1.93918

A26 1.93835 0.00000 0.00000 -0.00001 -0.00001 1.93835

A27 1.88691 0.00000 0.00001 0.00000 0.00001 1.88692

A28 1.95318 0.00000 0.00001 -0.00001 0.00000 1.95318

A29 1.91590 0.00000 -0.00002 0.00000 -0.00002 1.91588

A30 1.91725 0.00000 0.00001 0.00001 0.00001 1.91726

A31 1.90684 0.00000 0.00002 0.00000 0.00002 1.90685

A32 1.90843 0.00000 -0.00001 -0.00001 -0.00002 1.90842

A33 1.85986 0.00000 0.00000 0.00001 0.00001 1.85986

A34 1.96584 0.00000 0.00000 0.00000 0.00000 1.96584

A35 1.90636 0.00000 0.00001 0.00000 0.00000 1.90636

A36 1.90782 0.00000 0.00000 0.00000 0.00000 1.90783

A37 1.91283 0.00000 0.00002 0.00000 0.00002 1.91285

A38 1.91284 0.00000 -0.00002 -0.00001 -0.00002 1.91281

A39 1.85483 0.00000 0.00000 0.00000 0.00000 1.85483

A40 1.94555 0.00000 0.00000 -0.00001 0.00000 1.94555

A41 1.94205 0.00000 0.00001 0.00000 0.00001 1.94206

A42 1.94266 0.00000 0.00000 0.00000 0.00000 1.94266

A43 1.87711 0.00000 -0.00001 -0.00001 -0.00002 1.87709

A44 1.87715 0.00000 0.00000 0.00001 0.00001 1.87716

A45 1.87596 0.00000 0.00000 0.00000 0.00000 1.87595

D1 2.68590 0.00000 0.00002 0.00010 0.00012 2.68602

D2 -1.44030 0.00000 0.00004 0.00011 0.00015 -1.44015

D3 0.50273 0.00000 0.00000 0.00010 0.00010 0.50283

D4 -0.49163 0.00000 0.00008 0.00009 0.00017 -0.49146

D5 1.66535 0.00000 0.00010 0.00010 0.00020 1.66555

D6 -2.67481 0.00000 0.00006 0.00009 0.00015 -2.67466

D7 -3.10034 0.00000 -0.00012 0.00011 0.00000 -3.10034

D8 0.00642 0.00000 -0.00006 0.00010 0.00004 0.00646

D9 3.14112 0.00000 -0.00006 -0.00007 -0.00013 3.14099

D10 -1.07007 0.00000 -0.00006 -0.00010 -0.00016 -1.07023

D11 1.03927 0.00000 -0.00007 -0.00008 -0.00015 1.03912

D12 1.04535 0.00000 -0.00006 -0.00009 -0.00015 1.04520

D13 3.11734 0.00000 -0.00006 -0.00012 -0.00018 3.11716

D14 -1.05650 0.00000 -0.00007 -0.00011 -0.00018 -1.05668

D15 -0.99410 0.00000 -0.00009 -0.00006 -0.00015 -0.99425

D16 1.07789 0.00000 -0.00009 -0.00009 -0.00018 1.07771

D17 -3.09595 0.00000 -0.00010 -0.00007 -0.00018 -3.09613

D18 -3.08681 0.00000 -0.00023 -0.00012 -0.00036 -3.08717

D19 -0.87989 0.00000 -0.00023 -0.00011 -0.00033 -0.88023

D20 1.22448 0.00000 -0.00017 -0.00013 -0.00030 1.22418

D21 1.81816 0.00000 0.00002 -0.00009 -0.00007 1.81809

D22 -1.14185 0.00000 -0.00001 -0.00002 -0.00003 -1.14188

D23 2.59896 0.00000 0.00008 0.00009 0.00017 2.59913

D24 -0.72569 0.00000 0.00010 0.00002 0.00013 -0.72556

D25 -3.03598 0.00000 0.00001 0.00008 0.00009 -3.03589

D26 -0.91638 0.00000 0.00002 0.00010 0.00012 -0.91626

D27 1.12115 0.00000 0.00003 0.00009 0.00013 1.12128

D28 -3.12545 0.00000 -0.00004 0.00006 0.00002 -3.12543

D29 -1.00514 0.00000 -0.00003 0.00005 0.00002 -1.00512

D30 1.03447 0.00000 -0.00004 0.00007 0.00003 1.03450

D31 1.07370 0.00000 -0.00007 0.00007 0.00000 1.07370

D32 -3.08917 0.00000 -0.00006 0.00006 0.00000 -3.08917

D33 -1.04956 0.00000 -0.00007 0.00008 0.00001 -1.04956

D34 -1.02729 0.00000 -0.00008 0.00005 -0.00002 -1.02731

D35 1.09302 0.00000 -0.00006 0.00005 -0.00002 1.09301

D36 3.13263 0.00000 -0.00008 0.00006 -0.00001 3.13262

D37 -3.13332 0.00000 -0.00004 0.00004 0.00000 -3.13332

D38 -1.00360 0.00000 -0.00002 0.00004 0.00003 -1.00358

D39 1.01909 0.00000 -0.00002 0.00005 0.00003 1.01912

D40 1.02434 0.00000 -0.00003 0.00005 0.00001 1.02435

D41 -3.12913 0.00000 -0.00001 0.00005 0.00004 -3.12909

D42 -1.10643 0.00000 -0.00001 0.00005 0.00005 -1.10639

D43 -1.00499 0.00000 -0.00003 0.00004 0.00001 -1.00499

D44 1.12472 0.00000 -0.00001 0.00004 0.00003 1.12476

D45 -3.13577 0.00000 -0.00001 0.00005 0.00004 -3.13573

D46 3.13746 0.00000 -0.00004 -0.00004 -0.00008 3.13738

D47 -1.05035 0.00000 -0.00004 -0.00005 -0.00009 -1.05044

D48 1.04161 0.00000 -0.00004 -0.00004 -0.00008 1.04153

D49 1.01140 0.00000 -0.00006 -0.00003 -0.00010 1.01131

D50 3.10678 0.00000 -0.00006 -0.00005 -0.00011 3.10667

D51 -1.08444 0.00000 -0.00006 -0.00004 -0.00010 -1.08455

D52 -1.01779 0.00000 -0.00006 -0.00004 -0.00010 -1.01789

D53 1.07759 0.00000 -0.00006 -0.00005 -0.00011 1.07748

D54 -3.11364 0.00000 -0.00006 -0.00004 -0.00010 -3.11374

Item Value Threshold Converged?

Maximum Force 0.000017 0.000450 YES

RMS Force 0.000003 0.000300 YES

Maximum Displacement 0.001198 0.001800 YES

RMS Displacement 0.000315 0.001200 YES

Predicted change in Energy=-3.136479D-09

Optimization completed.

-- Stationary point found.

----------------------------

! Optimized Parameters !

! (Angstroms and Degrees) !

-------------------------- --------------------------

! Name Definition Value Derivative Info. !

--------------------------------------------------------------------------------

! R1 R(1,2) 1.5006 -DE/DX = 0.0 !

! R2 R(1,3) 1.2115 -DE/DX = 0.0 !

! R3 R(1,4) 1.3512 -DE/DX = 0.0 !

! R4 R(2,5) 1.5163 -DE/DX = 0.0 !

! R5 R(2,6) 1.911 -DE/DX = 0.0 !

! R6 R(2,14) 1.089 -DE/DX = 0.0 !

! R7 R(4,15) 0.972 -DE/DX = 0.0 !

! R8 R(5,16) 1.0908 -DE/DX = 0.0 !

! R9 R(5,17) 1.0947 -DE/DX = 0.0 !

! R10 R(5,18) 1.0901 -DE/DX = 0.0 !

! R11 R(6,7) 1.7543 -DE/DX = 0.0 !

! R12 R(7,8) 1.793 -DE/DX = 0.0 !

! R13 R(7,9) 1.7218 -DE/DX = 0.0 !

! R14 R(8,10) 1.8373 -DE/DX = 0.0 !

! R15 R(10,11) 1.5248 -DE/DX = 0.0 !

! R16 R(10,19) 1.0924 -DE/DX = 0.0 !

! R17 R(10,20) 1.0901 -DE/DX = 0.0 !

! R18 R(11,12) 1.5315 -DE/DX = 0.0 !

! R19 R(11,21) 1.0965 -DE/DX = 0.0 !

! R20 R(11,22) 1.096 -DE/DX = 0.0 !

! R21 R(12,13) 1.5274 -DE/DX = 0.0 !

! R22 R(12,23) 1.0964 -DE/DX = 0.0 !

! R23 R(12,24) 1.0964 -DE/DX = 0.0 !

! R24 R(13,25) 1.0941 -DE/DX = 0.0 !

! R25 R(13,26) 1.095 -DE/DX = 0.0 !

! R26 R(13,27) 1.0949 -DE/DX = 0.0 !

! A1 A(2,1,3) 124.7194 -DE/DX = 0.0 !

! A2 A(2,1,4) 113.2469 -DE/DX = 0.0 !

! A3 A(3,1,4) 122.0007 -DE/DX = 0.0 !

! A4 A(1,2,5) 116.0721 -DE/DX = 0.0 !

! A5 A(1,2,6) 104.9219 -DE/DX = 0.0 !

! A6 A(1,2,14) 107.3231 -DE/DX = 0.0 !

! A7 A(5,2,6) 111.5287 -DE/DX = 0.0 !

! A8 A(5,2,14) 111.2255 -DE/DX = 0.0 !

! A9 A(6,2,14) 104.9997 -DE/DX = 0.0 !

! A10 A(1,4,15) 107.32 -DE/DX = 0.0 !

! A11 A(2,5,16) 109.6036 -DE/DX = 0.0 !

! A12 A(2,5,17) 110.3603 -DE/DX = 0.0 !

! A13 A(2,5,18) 111.8579 -DE/DX = 0.0 !

! A14 A(16,5,17) 107.9158 -DE/DX = 0.0 !

! A15 A(16,5,18) 108.5346 -DE/DX = 0.0 !

! A16 A(17,5,18) 108.4658 -DE/DX = 0.0 !

! A17 A(2,6,7) 103.0605 -DE/DX = 0.0 !

! A18 A(6,7,8) 112.8171 -DE/DX = 0.0 !

! A19 A(6,7,9) 122.8027 -DE/DX = 0.0 !

! A20 A(8,7,9) 123.5005 -DE/DX = 0.0 !

! A21 A(7,8,10) 102.9302 -DE/DX = 0.0 !

! A22 A(8,10,11) 110.3575 -DE/DX = 0.0 !

! A23 A(8,10,19) 107.7089 -DE/DX = 0.0 !

! A24 A(8,10,20) 108.3795 -DE/DX = 0.0 !

! A25 A(11,10,19) 111.1058 -DE/DX = 0.0 !

! A26 A(11,10,20) 111.0593 -DE/DX = 0.0 !

! A27 A(19,10,20) 108.1119 -DE/DX = 0.0 !

! A28 A(10,11,12) 111.9091 -DE/DX = 0.0 !

! A29 A(10,11,21) 109.7731 -DE/DX = 0.0 !

! A30 A(10,11,22) 109.8501 -DE/DX = 0.0 !

! A31 A(12,11,21) 109.2538 -DE/DX = 0.0 !

! A32 A(12,11,22) 109.3452 -DE/DX = 0.0 !

! A33 A(21,11,22) 106.562 -DE/DX = 0.0 !

! A34 A(11,12,13) 112.6343 -DE/DX = 0.0 !

! A35 A(11,12,23) 109.2261 -DE/DX = 0.0 !

! A36 A(11,12,24) 109.3103 -DE/DX = 0.0 !

! A37 A(13,12,23) 109.5971 -DE/DX = 0.0 !

! A38 A(13,12,24) 109.5975 -DE/DX = 0.0 !

! A39 A(23,12,24) 106.274 -DE/DX = 0.0 !

! A40 A(12,13,25) 111.472 -DE/DX = 0.0 !

! A41 A(12,13,26) 111.2712 -DE/DX = 0.0 !

! A42 A(12,13,27) 111.306 -DE/DX = 0.0 !

! A43 A(25,13,26) 107.5502 -DE/DX = 0.0 !

! A44 A(25,13,27) 107.5527 -DE/DX = 0.0 !

! A45 A(26,13,27) 107.4844 -DE/DX = 0.0 !

! D1 D(3,1,2,5) 153.891 -DE/DX = 0.0 !

! D2 D(3,1,2,6) -82.523 -DE/DX = 0.0 !

! D3 D(3,1,2,14) 28.8041 -DE/DX = 0.0 !

! D4 D(4,1,2,5) -28.1683 -DE/DX = 0.0 !

! D5 D(4,1,2,6) 95.4177 -DE/DX = 0.0 !

! D6 D(4,1,2,14) -153.2552 -DE/DX = 0.0 !

! D7 D(2,1,4,15) -177.6363 -DE/DX = 0.0 !

! D8 D(3,1,4,15) 0.3678 -DE/DX = 0.0 !

! D9 D(1,2,5,16) 179.9729 -DE/DX = 0.0 !

! D10 D(1,2,5,17) -61.3103 -DE/DX = 0.0 !

! D11 D(1,2,5,18) 59.5457 -DE/DX = 0.0 !

! D12 D(6,2,5,16) 59.894 -DE/DX = 0.0 !

! D13 D(6,2,5,17) 178.6107 -DE/DX = 0.0 !

! D14 D(6,2,5,18) -60.5333 -DE/DX = 0.0 !

! D15 D(14,2,5,16) -56.9579 -DE/DX = 0.0 !

! D16 D(14,2,5,17) 61.7588 -DE/DX = 0.0 !

! D17 D(14,2,5,18) -177.3851 -DE/DX = 0.0 !

! D18 D(1,2,6,7) -176.8613 -DE/DX = 0.0 !

! D19 D(5,2,6,7) -50.4143 -DE/DX = 0.0 !

! D20 D(14,2,6,7) 70.1577 -DE/DX = 0.0 !

! D21 D(2,6,7,8) 104.1729 -DE/DX = 0.0 !

! D22 D(2,6,7,9) -65.423 -DE/DX = 0.0 !

! D23 D(6,7,8,10) 148.9094 -DE/DX = 0.0 !

! D24 D(9,7,8,10) -41.5788 -DE/DX = 0.0 !

! D25 D(7,8,10,11) -173.9489 -DE/DX = 0.0 !

! D26 D(7,8,10,19) -52.5047 -DE/DX = 0.0 !

! D27 D(7,8,10,20) 64.2373 -DE/DX = 0.0 !

! D28 D(8,10,11,12) -179.0752 -DE/DX = 0.0 !

! D29 D(8,10,11,21) -57.5903 -DE/DX = 0.0 !

! D30 D(8,10,11,22) 59.2707 -DE/DX = 0.0 !

! D31 D(19,10,11,12) 61.5187 -DE/DX = 0.0 !

! D32 D(19,10,11,21) -176.9964 -DE/DX = 0.0 !

! D33 D(19,10,11,22) -60.1355 -DE/DX = 0.0 !

! D34 D(20,10,11,12) -58.8592 -DE/DX = 0.0 !

! D35 D(20,10,11,21) 62.6257 -DE/DX = 0.0 !

! D36 D(20,10,11,22) 179.4866 -DE/DX = 0.0 !

! D37 D(10,11,12,13) -179.5261 -DE/DX = 0.0 !

! D38 D(10,11,12,23) -57.5022 -DE/DX = 0.0 !

! D39 D(10,11,12,24) 58.3897 -DE/DX = 0.0 !

! D40 D(21,11,12,13) 58.6904 -DE/DX = 0.0 !

! D41 D(21,11,12,23) -179.2858 -DE/DX = 0.0 !

! D42 D(21,11,12,24) -63.3938 -DE/DX = 0.0 !

! D43 D(22,11,12,13) -57.5819 -DE/DX = 0.0 !

! D44 D(22,11,12,23) 64.4419 -DE/DX = 0.0 !

! D45 D(22,11,12,24) -179.6661 -DE/DX = 0.0 !

! D46 D(11,12,13,25) 179.763 -DE/DX = 0.0 !

! D47 D(11,12,13,26) -60.1808 -DE/DX = 0.0 !

! D48 D(11,12,13,27) 59.6799 -DE/DX = 0.0 !

! D49 D(23,12,13,25) 57.9491 -DE/DX = 0.0 !

! D50 D(23,12,13,26) 178.0053 -DE/DX = 0.0 !

! D51 D(23,12,13,27) -62.1341 -DE/DX = 0.0 !

! D52 D(24,12,13,25) -58.3151 -DE/DX = 0.0 !

! D53 D(24,12,13,26) 61.7411 -DE/DX = 0.0 !

! D54 D(24,12,13,27) -178.3982 -DE/DX = 0.0 !

--------------------------------------------------------------------------------

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Largest change from initial coordinates is atom 16 0.166 Angstoms.

Leave Link 103 at Sat Aug 17 18:01:48 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.096935 -0.407372 -0.195158

2 6 0 -2.843703 0.074816 0.474591

3 8 0 -4.911410 0.309935 -0.733499

4 8 0 -4.223478 -1.752543 -0.184737

5 6 0 -2.291418 -0.812549 1.573116

6 16 0 -1.583521 0.301258 -0.944007

7 6 0 -0.118874 0.773273 -0.101607

8 16 0 1.079316 -0.556027 0.007943

9 16 0 0.022245 2.253773 0.765995

10 6 0 2.685567 0.335885 -0.008841

11 6 0 3.842235 -0.655647 -0.071961

12 6 0 5.201249 0.050444 -0.064723

13 6 0 6.372139 -0.927464 -0.139170

14 1 0 -3.038853 1.081381 0.841578

15 1 0 -5.037424 -1.970389 -0.669341

16 1 0 -1.385567 -0.365127 1.984265

17 1 0 -3.018139 -0.909261 2.386079

18 1 0 -2.049348 -1.809997 1.205904

19 1 0 2.688265 0.999207 -0.876788

20 1 0 2.746126 0.951803 0.888592

21 1 0 3.787783 -1.343864 0.779977

22 1 0 3.757014 -1.269860 -0.975715

23 1 0 5.250289 0.747823 -0.909342

24 1 0 5.288302 0.659962 0.842419

25 1 0 7.332531 -0.403250 -0.136990

26 1 0 6.369686 -1.615681 0.712515

27 1 0 6.328083 -1.532167 -1.050873

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.500553 0.000000

3 O 1.211491 2.406278 0.000000

4 O 1.351150 2.382799 2.242366 0.000000

5 C 2.559463 1.516308 3.666715 2.776056 0.000000

6 S 2.716649 1.910957 3.334552 3.429863 2.842111

7 C 4.150619 2.871330 4.856168 4.820210 3.168513

8 S 5.182366 4.000725 6.098231 5.439522 3.725240

9 S 4.997314 3.611984 5.510711 5.914442 3.925151

10 C 6.825648 5.556499 7.631504 7.219929 5.347136

11 C 7.944007 6.747893 8.831551 8.140739 6.352370

12 C 9.310361 8.063045 10.138070 9.596387 7.717987

13 C 10.482134 9.290479 11.366743 10.627790 8.831893

14 H 2.100177 1.089007 2.565632 3.238485 2.163510

15 H 1.884779 3.209962 2.284704 0.972011 3.729578

16 H 3.478963 2.144488 4.502613 3.831870 1.090778

17 H 2.842266 2.156993 3.847425 2.961935 1.094708

18 H 2.850078 2.172174 4.055465 2.581477 1.090112

19 H 6.962903 5.769176 7.632214 7.471496 5.837956

20 H 7.060408 5.673332 7.853727 7.552543 5.381297

21 H 7.999793 6.788411 8.983408 8.079480 6.153702

22 H 7.939627 6.890646 8.814533 8.034108 6.579453

23 H 9.445376 8.238987 10.172649 9.824924 8.091643

24 H 9.502549 8.161323 10.326672 9.866569 7.755924

25 H 11.429615 10.205798 12.279192 11.634613 9.783271

26 H 10.575161 9.370214 11.535253 10.631976 8.740730

27 H 10.520380 9.435628 11.393869 10.589343 9.038748

6 7 8 9 10

6 S 0.000000

7 C 1.754316 0.000000

8 S 2.954970 1.792958 0.000000

9 S 3.052033 1.721780 3.096291 0.000000

10 C 4.370451 2.839860 1.837343 3.372232 0.000000

11 C 5.578079 4.211067 2.765869 4.874343 1.524795

12 C 6.846105 5.369130 4.166943 5.689186 2.532440

13 C 8.090120 6.710229 5.307879 7.159661 3.899211

14 H 2.432056 3.083958 4.509475 3.278801 5.835063

15 H 4.143099 5.660577 6.314558 6.745664 8.087011

16 H 3.009657 2.692829 3.165113 3.213216 4.586723

17 H 3.822690 4.174354 4.750730 4.676899 6.310173

18 H 3.049018 3.479885 3.577162 4.582494 5.338524

19 H 4.328950 2.920956 2.406287 3.373475 1.092398

20 H 4.746312 3.036544 2.413990 3.021537 1.090142

21 H 5.876177 4.530059 2.924469 5.207923 2.158395

22 H 5.566932 4.467770 2.940614 5.421996 2.158995

23 H 6.848472 5.429640 4.465249 5.692722 2.749253

24 H 7.109286 5.490135 4.459882 5.502493 2.757517

25 H 8.980178 7.543799 6.256760 7.830418 4.707125

26 H 8.346988 6.962134 5.441259 7.434080 4.231039

27 H 8.121966 6.912266 5.442747 7.576143 4.224141

11 12 13 14 15

11 C 0.000000

12 C 1.531513 0.000000

13 C 2.545351 1.527360 0.000000

14 H 7.155501 8.353651 9.672853 0.000000

15 H 8.996319 10.453695 11.469390 3.948476 0.000000

16 H 5.625156 6.910658 8.062704 2.476181 4.791091

17 H 7.291845 8.630515 9.723915 2.519636 3.813017

18 H 6.138096 7.592555 8.573770 3.077649 3.531412

19 H 2.172080 2.806187 4.222211 5.979917 8.279360

20 H 2.169795 2.783682 4.211401 5.786621 8.458724

21 H 1.096543 2.157660 2.774367 7.244899 8.965341

22 H 1.096034 2.158453 2.766933 7.417189 8.827613

23 H 2.157208 1.096413 2.158309 8.478611 10.643463

24 H 2.158246 1.096357 2.158272 8.337811 10.762193

25 H 3.500014 2.180235 1.094148 10.522705 12.480189

26 H 2.815150 2.178374 1.094996 9.788329 11.495977

27 H 2.811760 2.178739 1.094902 9.907143 11.380349

16 17 18 19 20

16 H 0.000000

17 H 1.767152 0.000000

18 H 1.770339 1.772764 0.000000

19 H 5.161700 6.844822 5.888481 0.000000

20 H 4.472772 6.239613 5.542996 1.766964 0.000000

21 H 5.401091 7.006355 5.871184 3.073075 2.523278

22 H 6.002180 7.571947 6.226159 2.510114 3.071371

23 H 7.324357 9.053873 8.018816 2.574532 3.089499

24 H 6.848003 8.593154 7.750738 3.135435 2.559289

25 H 8.972537 10.665753 9.581334 4.907484 4.891124

26 H 7.957712 9.561960 8.435717 4.787105 4.444452

27 H 8.371048 9.977600 8.680529 4.436939 4.770958

21 22 23 24 25

21 H 0.000000

22 H 1.757520 0.000000

23 H 3.060698 2.511039 0.000000

24 H 2.504151 3.061808 1.754375 0.000000

25 H 3.780320 3.773433 2.501446 2.503705 0.000000

26 H 2.597047 3.129818 3.077274 2.522859 1.765990

27 H 3.136972 2.585507 2.525871 3.077520 1.765943

26 27

26 H 0.000000

27 H 1.765854 0.000000

Stoichiometry C8H14O2S3(1-,2)

Framework group C1[X(C8H14O2S3)]

Deg. of freedom 75

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.22D-15

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.104244 -0.467221 -0.120176

2 6 0 -2.846184 0.116694 0.452526

3 8 0 -4.922633 0.153170 -0.762877

4 8 0 -4.230673 -1.792369 0.111350

5 6 0 -2.285898 -0.579397 1.677568

6 16 0 -1.596364 0.106249 -0.993017

7 6 0 -0.125639 0.708162 -0.249851

8 16 0 1.073352 -0.586637 0.067349

9 16 0 0.021751 2.310610 0.362492

10 6 0 2.679415 0.288606 -0.106839

11 6 0 3.835619 -0.701221 -0.015000

12 6 0 5.194631 -0.005067 -0.133278

13 6 0 6.364974 -0.983326 -0.054946

14 1 0 -3.038685 1.170002 0.651074

15 1 0 -5.048118 -2.085699 -0.325167

16 1 0 -1.377091 -0.071731 2.003361

17 1 0 -3.006681 -0.540796 2.500591

18 1 0 -2.046480 -1.623803 1.476969

19 1 0 2.675780 0.800800 -1.071711

20 1 0 2.746486 1.043129 0.677129

21 1 0 3.787385 -1.240537 0.938530

22 1 0 3.743840 -1.455069 -0.805304

23 1 0 5.237506 0.544492 -1.081049

24 1 0 5.288266 0.744703 0.661125

25 1 0 7.325343 -0.466955 -0.145559

26 1 0 6.368735 -1.522743 0.897960

27 1 0 6.314301 -1.729143 -0.854946

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3037965 0.1935949 0.1808827

Leave Link 202 at Sat Aug 17 18:01:48 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l601.exe)

Copying SCF densities to generalized density rwf, IOpCl= 1 IROHF=0.

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Population analysis using the SCF density.

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Orbital symmetries:

Alpha Orbitals:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

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Beta Orbitals:

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The electronic state is 2-A.

Alpha occ. eigenvalues -- -88.83212 -88.82871 -88.77127 -19.16009 -19.10150

Alpha occ. eigenvalues -- -10.29762 -10.20649 -10.19877 -10.17612 -10.15782

Alpha occ. eigenvalues -- -10.15544 -10.15248 -10.14683 -7.91761 -7.91450

Alpha occ. eigenvalues -- -7.85748 -5.88152 -5.87803 -5.87769 -5.87443

Alpha occ. eigenvalues -- -5.87164 -5.86954 -5.82094 -5.81755 -5.81327

Alpha occ. eigenvalues -- -1.10583 -1.01388 -0.82095 -0.80108 -0.77347

Alpha occ. eigenvalues -- -0.73337 -0.68101 -0.66449 -0.65316 -0.60754

Alpha occ. eigenvalues -- -0.58743 -0.57218 -0.49664 -0.48368 -0.47506

Alpha occ. eigenvalues -- -0.46958 -0.45091 -0.42462 -0.42055 -0.41728

Alpha occ. eigenvalues -- -0.40842 -0.39699 -0.38594 -0.37653 -0.36569

Alpha occ. eigenvalues -- -0.35935 -0.35430 -0.33805 -0.32831 -0.32471

Alpha occ. eigenvalues -- -0.32108 -0.31937 -0.29543 -0.27864 -0.27021

Alpha occ. eigenvalues -- -0.22843 -0.21290 -0.18715 -0.12763

Alpha virt. eigenvalues -- -0.00660 0.02861 0.04222 0.05253 0.06092

Alpha virt. eigenvalues -- 0.06950 0.07701 0.08505 0.08665 0.09235

Alpha virt. eigenvalues -- 0.10226 0.10499 0.11334 0.12457 0.13338

Alpha virt. eigenvalues -- 0.14281 0.14705 0.14948 0.15253 0.16867

Alpha virt. eigenvalues -- 0.17936 0.19157 0.20675 0.21081 0.22474

Alpha virt. eigenvalues -- 0.22700 0.24168 0.24276 0.24737 0.25441

Alpha virt. eigenvalues -- 0.26483 0.27239 0.27983 0.30415 0.30556

Alpha virt. eigenvalues -- 0.31352 0.32237 0.33753 0.34244 0.35177

Alpha virt. eigenvalues -- 0.36194 0.36643 0.37663 0.38432 0.41119

Alpha virt. eigenvalues -- 0.41918 0.44726 0.45044 0.48115 0.48835

Alpha virt. eigenvalues -- 0.49368 0.50937 0.52619 0.53565 0.54042

Alpha virt. eigenvalues -- 0.55977 0.56849 0.57384 0.59069 0.59548

Alpha virt. eigenvalues -- 0.59850 0.60054 0.60281 0.60733 0.61903

Alpha virt. eigenvalues -- 0.62163 0.62400 0.62817 0.63047 0.63465

Alpha virt. eigenvalues -- 0.64067 0.64175 0.66463 0.67041 0.67729

Alpha virt. eigenvalues -- 0.69307 0.69997 0.72974 0.75671 0.76970

Alpha virt. eigenvalues -- 0.79156 0.80059 0.81018 0.82084 0.83548

Alpha virt. eigenvalues -- 0.84520 0.86450 0.88621 0.89706 0.91226

Alpha virt. eigenvalues -- 0.91893 0.92869 0.93948 0.94904 0.96153

Alpha virt. eigenvalues -- 0.97614 0.98293 0.99585 1.01305 1.02519

Alpha virt. eigenvalues -- 1.05424 1.08012 1.09340 1.11446 1.13246

Alpha virt. eigenvalues -- 1.14815 1.18048 1.18941 1.19437 1.24777

Alpha virt. eigenvalues -- 1.32058 1.35443 1.39419 1.44250 1.46742

Alpha virt. eigenvalues -- 1.47042 1.47980 1.48761 1.50917 1.52202

Alpha virt. eigenvalues -- 1.53174 1.53700 1.54572 1.55702 1.58795

Alpha virt. eigenvalues -- 1.59324 1.62754 1.63363 1.63969 1.65401

Alpha virt. eigenvalues -- 1.65795 1.66302 1.67350 1.67923 1.69726

Alpha virt. eigenvalues -- 1.70867 1.72795 1.75274 1.77678 1.79592

Alpha virt. eigenvalues -- 1.80600 1.81358 1.83477 1.86738 1.87498

Alpha virt. eigenvalues -- 1.89728 1.90974 1.91964 1.94452 1.96218

Alpha virt. eigenvalues -- 1.97900 1.98855 2.01019 2.06338 2.12004

Alpha virt. eigenvalues -- 2.15871 2.18232 2.20790 2.37832 2.39554

Alpha virt. eigenvalues -- 2.39906 2.41903 2.42354 2.43794 2.44248

Alpha virt. eigenvalues -- 2.47691 2.50336 2.50978 2.52213 2.53163

Alpha virt. eigenvalues -- 2.54878 2.59003 2.74264 2.77563 2.84782

Alpha virt. eigenvalues -- 2.85399 2.87698 2.91378 2.92598 2.94431

Alpha virt. eigenvalues -- 2.98358 3.01279 3.03239 3.07085 3.09029

Alpha virt. eigenvalues -- 3.11345 3.11777 3.13395 3.15281 3.15649

Alpha virt. eigenvalues -- 3.19024 3.20461 3.20820 3.23433 3.26446

Alpha virt. eigenvalues -- 3.33202 3.34597 3.51417 3.56657 3.62642

Alpha virt. eigenvalues -- 3.71578 3.86100 3.88256 4.05160 4.07766

Alpha virt. eigenvalues -- 4.80293 4.91248 4.96805 5.08390 5.37551

Alpha virt. eigenvalues -- 5.67768 7.70507 7.82555 7.85698 17.28040

Alpha virt. eigenvalues -- 17.30380 17.30578 17.33374 17.37378 17.41432

Alpha virt. eigenvalues -- 17.44557 17.45872 17.50227 23.36953 23.40214

Alpha virt. eigenvalues -- 23.47649 23.56681 23.67549 23.69952 23.73318

Alpha virt. eigenvalues -- 23.78432 49.81913 49.98653 188.83162 188.95822

Alpha virt. eigenvalues -- 189.00129

Beta occ. eigenvalues -- -88.83213 -88.82824 -88.76994 -19.15994 -19.10115

Beta occ. eigenvalues -- -10.29740 -10.19753 -10.19708 -10.17590 -10.15782

Beta occ. eigenvalues -- -10.15544 -10.15254 -10.14683 -7.91756 -7.91408

Beta occ. eigenvalues -- -7.85629 -5.88176 -5.87796 -5.87785 -5.87426

Beta occ. eigenvalues -- -5.87125 -5.86792 -5.82043 -5.81321 -5.81251

Beta occ. eigenvalues -- -1.10537 -1.01330 -0.81483 -0.79985 -0.76837

Beta occ. eigenvalues -- -0.72974 -0.67961 -0.66241 -0.64894 -0.60552

Beta occ. eigenvalues -- -0.58616 -0.57189 -0.48755 -0.48217 -0.47389

Beta occ. eigenvalues -- -0.46925 -0.44686 -0.42341 -0.41919 -0.41648

Beta occ. eigenvalues -- -0.40664 -0.39448 -0.38441 -0.37387 -0.36418

Beta occ. eigenvalues -- -0.35599 -0.35253 -0.33467 -0.32452 -0.32100

Beta occ. eigenvalues -- -0.32053 -0.31445 -0.29153 -0.27557 -0.25317

Beta occ. eigenvalues -- -0.22513 -0.19824 -0.18375

Beta virt. eigenvalues -- -0.05064 0.00483 0.03506 0.04553 0.05425

Beta virt. eigenvalues -- 0.06292 0.07295 0.07767 0.08612 0.08875

Beta virt. eigenvalues -- 0.09448 0.10430 0.10686 0.11408 0.12501

Beta virt. eigenvalues -- 0.13435 0.14356 0.14731 0.14999 0.15285

Beta virt. eigenvalues -- 0.16929 0.18044 0.19449 0.20759 0.21361

Beta virt. eigenvalues -- 0.22705 0.22797 0.24341 0.24605 0.24847

Beta virt. eigenvalues -- 0.25606 0.26680 0.27575 0.28240 0.30483

Beta virt. eigenvalues -- 0.30794 0.31422 0.32511 0.33993 0.34308

Beta virt. eigenvalues -- 0.35280 0.36309 0.36735 0.37735 0.38561

Beta virt. eigenvalues -- 0.41231 0.42119 0.45061 0.45177 0.48469

Beta virt. eigenvalues -- 0.49255 0.49555 0.51188 0.52924 0.53688

Beta virt. eigenvalues -- 0.54363 0.56203 0.57039 0.57679 0.59194

Beta virt. eigenvalues -- 0.59565 0.59922 0.60085 0.60363 0.61099

Beta virt. eigenvalues -- 0.61957 0.62367 0.62517 0.62901 0.63071

Beta virt. eigenvalues -- 0.63545 0.64185 0.64247 0.66741 0.67246

Beta virt. eigenvalues -- 0.67983 0.69805 0.70508 0.73319 0.75769

Beta virt. eigenvalues -- 0.77508 0.79280 0.80286 0.81591 0.82401

Beta virt. eigenvalues -- 0.83850 0.85022 0.87340 0.89228 0.89903

Beta virt. eigenvalues -- 0.91734 0.92343 0.93032 0.94226 0.95094

Beta virt. eigenvalues -- 0.96409 0.97775 0.98780 0.99849 1.01457

Beta virt. eigenvalues -- 1.03391 1.05585 1.08253 1.09612 1.11673

Beta virt. eigenvalues -- 1.13410 1.15060 1.18179 1.19057 1.19569

Beta virt. eigenvalues -- 1.24916 1.32124 1.35534 1.39442 1.44747

Beta virt. eigenvalues -- 1.46969 1.47927 1.48451 1.49003 1.51588

Beta virt. eigenvalues -- 1.52590 1.53406 1.54070 1.54950 1.56104

Beta virt. eigenvalues -- 1.58902 1.59458 1.62920 1.63477 1.64197

Beta virt. eigenvalues -- 1.65712 1.66037 1.66561 1.67613 1.68483

Beta virt. eigenvalues -- 1.70114 1.71460 1.73755 1.75617 1.78124

Beta virt. eigenvalues -- 1.79659 1.80889 1.81403 1.83837 1.87100

Beta virt. eigenvalues -- 1.87705 1.90016 1.91182 1.92260 1.94934

Beta virt. eigenvalues -- 1.96891 1.98040 1.99112 2.01291 2.06890

Beta virt. eigenvalues -- 2.12062 2.15990 2.18583 2.20861 2.37837

Beta virt. eigenvalues -- 2.39565 2.39916 2.41932 2.42387 2.43820

Beta virt. eigenvalues -- 2.44365 2.47770 2.50536 2.50989 2.52260

Beta virt. eigenvalues -- 2.53174 2.54893 2.59143 2.75348 2.79728

Beta virt. eigenvalues -- 2.85052 2.85848 2.87807 2.91416 2.92682

Beta virt. eigenvalues -- 2.94488 2.98494 3.01679 3.03641 3.07208

Beta virt. eigenvalues -- 3.09033 3.11571 3.11839 3.13980 3.15539

Beta virt. eigenvalues -- 3.15727 3.19065 3.20500 3.20863 3.23484

Beta virt. eigenvalues -- 3.26474 3.33276 3.34668 3.51473 3.56702

Beta virt. eigenvalues -- 3.62650 3.71677 3.86112 3.88278 4.05167

Beta virt. eigenvalues -- 4.07899 4.80361 4.91390 4.96837 5.08406

Beta virt. eigenvalues -- 5.37591 5.67797 7.70651 7.82721 7.85785

Beta virt. eigenvalues -- 17.28223 17.30665 17.30878 17.33499 17.37375

Beta virt. eigenvalues -- 17.41427 17.44605 17.45892 17.50285 23.37040

Beta virt. eigenvalues -- 23.41073 23.47764 23.56692 23.67556 23.70043

Beta virt. eigenvalues -- 23.73321 23.78502 49.81931 49.98687 188.83232

Beta virt. eigenvalues -- 188.95897 189.00153

Condensed to atoms (all electrons):

1 2 3 4 5 6

1 C 4.509605 0.287449 0.642490 0.309519 -0.034473 -0.051494

2 C 0.287449 5.776104 -0.092795 -0.101502 0.211228 0.145637

3 O 0.642490 -0.092795 7.873366 -0.089269 0.004577 0.010802

4 O 0.309519 -0.101502 -0.089269 8.115762 0.006184 0.006569

5 C -0.034473 0.211228 0.004577 0.006184 5.407340 -0.068363

6 S -0.051494 0.145637 0.010802 0.006569 -0.068363 15.956322

7 C 0.004047 -0.056337 -0.000008 -0.000033 -0.010396 0.273871

8 S -0.000107 -0.015129 0.000034 -0.000152 0.007102 -0.135545

9 S 0.000498 -0.007886 -0.000083 -0.000045 -0.007643 -0.143385

10 C 0.000000 -0.000055 0.000000 0.000000 -0.000043 -0.000325

11 C 0.000000 0.000000 0.000000 0.000000 0.000001 -0.000243

12 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000015

13 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

14 H -0.053540 0.381895 0.007827 0.004285 -0.048205 -0.069115

15 H -0.036320 0.015916 0.012941 0.245233 -0.001465 -0.001031

16 H 0.006620 -0.037967 -0.000193 0.000148 0.391066 -0.014236

17 H -0.004536 -0.034529 0.000114 0.001717 0.377096 0.010365

18 H -0.006882 -0.037496 0.000239 0.008383 0.384395 -0.003818

19 H 0.000000 0.000027 0.000000 0.000000 0.000002 0.004938

20 H 0.000000 -0.000019 0.000000 0.000000 -0.000003 -0.001670

21 H 0.000000 0.000000 0.000000 0.000000 -0.000002 0.000001

22 H 0.000000 -0.000001 0.000000 0.000000 0.000000 -0.000229

23 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000007

24 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000001

25 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

26 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

27 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

7 8 9 10 11 12

1 C 0.004047 -0.000107 0.000498 0.000000 0.000000 0.000000

2 C -0.056337 -0.015129 -0.007886 -0.000055 0.000000 0.000000

3 O -0.000008 0.000034 -0.000083 0.000000 0.000000 0.000000

4 O -0.000033 -0.000152 -0.000045 0.000000 0.000000 0.000000

5 C -0.010396 0.007102 -0.007643 -0.000043 0.000001 0.000000

6 S 0.273871 -0.135545 -0.143385 -0.000325 -0.000243 0.000015

7 C 6.038568 0.146046 0.212110 -0.046673 0.004130 -0.000213

8 S 0.146046 15.964556 -0.117170 0.209347 -0.057702 0.008703

9 S 0.212110 -0.117170 16.558334 -0.019642 0.002478 0.000328

10 C -0.046673 0.209347 -0.019642 5.517668 0.309569 -0.061663

11 C 0.004130 -0.057702 0.002478 0.309569 5.275737 0.323327

12 C -0.000213 0.008703 0.000328 -0.061663 0.323327 5.216687

13 C 0.000002 -0.000536 0.000004 0.006953 -0.070760 0.328477

14 H -0.009836 -0.000502 0.017667 0.000015 0.000000 0.000000

15 H 0.000042 0.000002 0.000004 0.000000 0.000000 0.000000

16 H 0.000787 -0.002779 0.002443 -0.000227 0.000000 0.000000

17 H 0.000102 0.000243 -0.000506 0.000000 0.000000 0.000000

18 H -0.001746 0.000097 0.001160 -0.000015 -0.000002 0.000000

19 H 0.004659 -0.064824 -0.003984 0.357539 -0.031153 -0.007920

20 H -0.008402 -0.067817 0.005835 0.374460 -0.035860 -0.005920

21 H -0.000062 0.001169 -0.000193 -0.043832 0.395995 -0.044395

22 H -0.000315 -0.001186 -0.000283 -0.041836 0.396109 -0.044463

23 H -0.000018 -0.000286 0.000082 -0.004755 -0.045725 0.399917

24 H 0.000012 -0.000101 -0.000071 -0.004469 -0.044707 0.398387

25 H 0.000000 0.000035 0.000000 -0.000333 0.008156 -0.037598

26 H 0.000000 -0.000034 0.000001 -0.000140 -0.005638 -0.038959

27 H 0.000000 -0.000013 -0.000001 -0.000142 -0.005671 -0.039195

13 14 15 16 17 18

1 C 0.000000 -0.053540 -0.036320 0.006620 -0.004536 -0.006882

2 C 0.000000 0.381895 0.015916 -0.037967 -0.034529 -0.037496

3 O 0.000000 0.007827 0.012941 -0.000193 0.000114 0.000239

4 O 0.000000 0.004285 0.245233 0.000148 0.001717 0.008383

5 C 0.000000 -0.048205 -0.001465 0.391066 0.377096 0.384395

6 S 0.000000 -0.069115 -0.001031 -0.014236 0.010365 -0.003818

7 C 0.000002 -0.009836 0.000042 0.000787 0.000102 -0.001746

8 S -0.000536 -0.000502 0.000002 -0.002779 0.000243 0.000097

9 S 0.000004 0.017667 0.000004 0.002443 -0.000506 0.001160

10 C 0.006953 0.000015 0.000000 -0.000227 0.000000 -0.000015

11 C -0.070760 0.000000 0.000000 0.000000 0.000000 -0.000002

12 C 0.328477 0.000000 0.000000 0.000000 0.000000 0.000000

13 C 5.299439 0.000000 0.000000 0.000000 0.000000 0.000000

14 H 0.000000 0.501764 -0.000796 -0.007562 -0.001455 0.006612

15 H 0.000000 -0.000796 0.352517 0.000110 -0.000324 -0.000274

16 H 0.000000 -0.007562 0.000110 0.474240 -0.032664 -0.025047

17 H 0.000000 -0.001455 -0.000324 -0.032664 0.489460 -0.029720

18 H 0.000000 0.006612 -0.000274 -0.025047 -0.029720 0.478861

19 H 0.000018 0.000014 0.000000 -0.000022 0.000001 0.000002

20 H -0.000058 -0.000016 0.000000 0.000216 -0.000004 -0.000001

21 H -0.003163 0.000000 0.000000 -0.000003 0.000000 0.000000

22 H -0.003472 0.000000 0.000000 0.000004 0.000000 -0.000001

23 H -0.041395 0.000000 0.000000 0.000000 0.000000 0.000000

24 H -0.040848 0.000000 0.000000 0.000000 0.000000 0.000000

25 H 0.392060 0.000000 0.000000 0.000000 0.000000 0.000000

26 H 0.387125 0.000000 0.000000 0.000000 0.000000 0.000000

27 H 0.387346 0.000000 0.000000 0.000000 0.000000 0.000000

19 20 21 22 23 24

1 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

2 C 0.000027 -0.000019 0.000000 -0.000001 0.000000 0.000000

3 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

4 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

5 C 0.000002 -0.000003 -0.000002 0.000000 0.000000 0.000000

6 S 0.004938 -0.001670 0.000001 -0.000229 -0.000007 0.000001

7 C 0.004659 -0.008402 -0.000062 -0.000315 -0.000018 0.000012

8 S -0.064824 -0.067817 0.001169 -0.001186 -0.000286 -0.000101

9 S -0.003984 0.005835 -0.000193 -0.000283 0.000082 -0.000071

10 C 0.357539 0.374460 -0.043832 -0.041836 -0.004755 -0.004469

11 C -0.031153 -0.035860 0.395995 0.396109 -0.045725 -0.044707

12 C -0.007920 -0.005920 -0.044395 -0.044463 0.399917 0.398387

13 C 0.000018 -0.000058 -0.003163 -0.003472 -0.041395 -0.040848

14 H 0.000014 -0.000016 0.000000 0.000000 0.000000 0.000000

15 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

16 H -0.000022 0.000216 -0.000003 0.000004 0.000000 0.000000

17 H 0.000001 -0.000004 0.000000 0.000000 0.000000 0.000000

18 H 0.000002 -0.000001 0.000000 -0.000001 0.000000 0.000000

19 H 0.547518 -0.050388 0.008754 -0.006903 0.003441 -0.000283

20 H -0.050388 0.531105 -0.006519 0.008415 -0.000420 0.004160

21 H 0.008754 -0.006519 0.512520 -0.038004 0.008322 -0.007270

22 H -0.006903 0.008415 -0.038004 0.514063 -0.007171 0.008342

23 H 0.003441 -0.000420 0.008322 -0.007171 0.522730 -0.039887

24 H -0.000283 0.004160 -0.007270 0.008342 -0.039887 0.521652

25 H -0.000017 -0.000002 -0.000208 -0.000180 -0.004749 -0.004718

26 H -0.000015 0.000037 0.004393 -0.000425 0.008134 -0.006600

27 H 0.000060 -0.000010 -0.000393 0.004447 -0.006530 0.008097

25 26 27

1 C 0.000000 0.000000 0.000000

2 C 0.000000 0.000000 0.000000

3 O 0.000000 0.000000 0.000000

4 O 0.000000 0.000000 0.000000

5 C 0.000000 0.000000 0.000000

6 S 0.000000 0.000000 0.000000

7 C 0.000000 0.000000 0.000000

8 S 0.000035 -0.000034 -0.000013

9 S 0.000000 0.000001 -0.000001

10 C -0.000333 -0.000140 -0.000142

11 C 0.008156 -0.005638 -0.005671

12 C -0.037598 -0.038959 -0.039195

13 C 0.392060 0.387125 0.387346

14 H 0.000000 0.000000 0.000000

15 H 0.000000 0.000000 0.000000

16 H 0.000000 0.000000 0.000000

17 H 0.000000 0.000000 0.000000

18 H 0.000000 0.000000 0.000000

19 H -0.000017 -0.000015 0.000060

20 H -0.000002 0.000037 -0.000010

21 H -0.000208 0.004393 -0.000393

22 H -0.000180 -0.000425 0.004447

23 H -0.004749 0.008134 -0.006530

24 H -0.004718 -0.006600 0.008097

25 H 0.492638 -0.030110 -0.030168

26 H -0.030110 0.504021 -0.033344

27 H -0.030168 -0.033344 0.503909

Atomic-Atomic Spin Densities.

1 2 3 4 5 6

1 C 0.018963 0.006422 -0.005994 -0.003255 0.000903 -0.000167

2 C 0.006422 0.217196 -0.002078 -0.001714 -0.020311 -0.098115

3 O -0.005994 -0.002078 0.017864 0.000458 0.000008 0.001802

4 O -0.003255 -0.001714 0.000458 0.007886 0.000033 0.000356

5 C 0.000903 -0.020311 0.000008 0.000033 0.001508 0.006826

6 S -0.000167 -0.098115 0.001802 0.000356 0.006826 0.113173

7 C 0.000483 -0.032216 0.000000 0.000013 0.008238 0.034496

8 S -0.000047 -0.008351 0.000013 0.000039 0.000682 -0.014955

9 S -0.000629 0.010546 0.000025 0.000005 0.000253 -0.011943

10 C 0.000000 -0.000086 0.000000 0.000000 0.000028 -0.004635

11 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000010

12 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000023

13 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

14 H -0.002670 0.009318 0.000551 0.000125 -0.000952 -0.013511

15 H -0.000013 -0.000526 0.000083 -0.000208 0.000098 0.000588

16 H 0.000110 -0.001896 -0.000003 -0.000007 0.001372 0.001434

17 H -0.000777 -0.000330 0.000036 0.000153 0.001100 -0.001180

18 H -0.000196 0.001304 0.000000 0.000031 -0.000497 -0.000007

19 H 0.000000 0.000072 0.000000 0.000000 -0.000014 0.003196

20 H 0.000000 -0.000037 0.000000 0.000000 0.000014 -0.000860

21 H 0.000000 0.000001 0.000000 0.000000 -0.000001 0.000049

22 H 0.000000 -0.000001 0.000000 0.000000 0.000000 -0.000082

23 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000008

24 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000002

25 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

26 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

27 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

7 8 9 10 11 12

1 C 0.000483 -0.000047 -0.000629 0.000000 0.000000 0.000000

2 C -0.032216 -0.008351 0.010546 -0.000086 0.000000 0.000000

3 O 0.000000 0.000013 0.000025 0.000000 0.000000 0.000000

4 O 0.000013 0.000039 0.000005 0.000000 0.000000 0.000000

5 C 0.008238 0.000682 0.000253 0.000028 0.000000 0.000000

6 S 0.034496 -0.014955 -0.011943 -0.004635 -0.000010 -0.000023

7 C 0.796804 -0.087354 -0.191788 -0.013915 0.000176 -0.000045

8 S -0.087354 0.186272 0.023550 -0.007003 -0.002585 -0.001180

9 S -0.191788 0.023550 0.432200 0.006818 -0.000296 0.000117

10 C -0.013915 -0.007003 0.006818 0.037705 -0.000087 0.000800

11 C 0.000176 -0.002585 -0.000296 -0.000087 0.000531 -0.000828

12 C -0.000045 -0.001180 0.000117 0.000800 -0.000828 0.002051

13 C 0.000000 0.000077 -0.000003 0.000013 0.000077 -0.000355

14 H -0.004514 -0.000580 0.005859 -0.000012 0.000000 0.000000

15 H 0.000010 0.000016 -0.000009 0.000000 0.000000 0.000000

16 H 0.003303 -0.000335 -0.004801 0.000064 0.000003 0.000000

17 H -0.000508 -0.000047 0.000686 -0.000001 0.000000 0.000000

18 H -0.000784 0.000111 0.000277 -0.000008 0.000000 0.000000

19 H 0.014479 -0.001452 -0.012739 -0.019130 0.003077 -0.002267

20 H -0.001608 -0.009047 0.002555 0.007678 -0.000274 0.001211

21 H 0.000023 0.002095 -0.000016 -0.000934 -0.000217 -0.000592

22 H -0.000107 -0.000240 0.000069 0.000715 -0.000062 0.000476

23 H -0.000022 -0.000093 0.000070 0.000112 -0.000440 0.000683

24 H 0.000004 0.000141 -0.000019 0.000013 0.000063 -0.000319

25 H 0.000000 -0.000005 0.000000 0.000000 -0.000018 0.000038

26 H 0.000000 -0.000023 0.000000 0.000001 0.000002 0.000083

27 H 0.000000 0.000018 -0.000001 -0.000008 0.000064 -0.000119

13 14 15 16 17 18

1 C 0.000000 -0.002670 -0.000013 0.000110 -0.000777 -0.000196

2 C 0.000000 0.009318 -0.000526 -0.001896 -0.000330 0.001304

3 O 0.000000 0.000551 0.000083 -0.000003 0.000036 0.000000

4 O 0.000000 0.000125 -0.000208 -0.000007 0.000153 0.000031

5 C 0.000000 -0.000952 0.000098 0.001372 0.001100 -0.000497

6 S 0.000000 -0.013511 0.000588 0.001434 -0.001180 -0.000007

7 C 0.000000 -0.004514 0.000010 0.003303 -0.000508 -0.000784

8 S 0.000077 -0.000580 0.000016 -0.000335 -0.000047 0.000111

9 S -0.000003 0.005859 -0.000009 -0.004801 0.000686 0.000277

10 C 0.000013 -0.000012 0.000000 0.000064 -0.000001 -0.000008

11 C 0.000077 0.000000 0.000000 0.000003 0.000000 0.000000

12 C -0.000355 0.000000 0.000000 0.000000 0.000000 0.000000

13 C 0.000408 0.000000 0.000000 0.000000 0.000000 0.000000

14 H 0.000000 0.003078 -0.000076 -0.000612 0.000750 0.000089

15 H 0.000000 -0.000076 0.000156 0.000004 -0.000031 -0.000025

16 H 0.000000 -0.000612 0.000004 0.000149 -0.000309 -0.000366

17 H 0.000000 0.000750 -0.000031 -0.000309 0.001571 0.000356

18 H 0.000000 0.000089 -0.000025 -0.000366 0.000356 0.000022

19 H 0.000102 0.000011 0.000000 -0.000017 0.000000 0.000003

20 H -0.000062 -0.000009 0.000000 0.000024 -0.000001 -0.000003

21 H 0.000112 0.000000 0.000000 -0.000002 0.000000 0.000000

22 H -0.000070 0.000000 0.000000 0.000000 0.000000 0.000000

23 H -0.000151 0.000000 0.000000 0.000000 0.000000 0.000000

24 H 0.000105 0.000000 0.000000 0.000000 0.000000 0.000000

25 H -0.000036 0.000000 0.000000 0.000000 0.000000 0.000000

26 H -0.000070 0.000000 0.000000 0.000000 0.000000 0.000000

27 H 0.000045 0.000000 0.000000 0.000000 0.000000 0.000000

19 20 21 22 23 24

1 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

2 C 0.000072 -0.000037 0.000001 -0.000001 0.000000 0.000000

3 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

4 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

5 C -0.000014 0.000014 -0.000001 0.000000 0.000000 0.000000

6 S 0.003196 -0.000860 0.000049 -0.000082 -0.000008 0.000002

7 C 0.014479 -0.001608 0.000023 -0.000107 -0.000022 0.000004

8 S -0.001452 -0.009047 0.002095 -0.000240 -0.000093 0.000141

9 S -0.012739 0.002555 -0.000016 0.000069 0.000070 -0.000019

10 C -0.019130 0.007678 -0.000934 0.000715 0.000112 0.000013

11 C 0.003077 -0.000274 -0.000217 -0.000062 -0.000440 0.000063

12 C -0.002267 0.001211 -0.000592 0.000476 0.000683 -0.000319

13 C 0.000102 -0.000062 0.000112 -0.000070 -0.000151 0.000105

14 H 0.000011 -0.000009 0.000000 0.000000 0.000000 0.000000

15 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

16 H -0.000017 0.000024 -0.000002 0.000000 0.000000 0.000000

17 H 0.000000 -0.000001 0.000000 0.000000 0.000000 0.000000

18 H 0.000003 -0.000003 0.000000 0.000000 0.000000 0.000000

19 H 0.027988 -0.006373 0.000448 -0.000659 -0.000723 0.000206

20 H -0.006373 0.005779 -0.000411 0.000182 0.000217 -0.000221

21 H 0.000448 -0.000411 0.000033 -0.000106 -0.000066 0.000069

22 H -0.000659 0.000182 -0.000106 -0.000059 0.000080 -0.000029

23 H -0.000723 0.000217 -0.000066 0.000080 0.000370 -0.000102

24 H 0.000206 -0.000221 0.000069 -0.000029 -0.000102 0.000186

25 H -0.000010 0.000005 -0.000009 0.000009 0.000041 -0.000020

26 H -0.000009 0.000009 -0.000032 0.000012 0.000015 -0.000017

27 H 0.000030 -0.000009 0.000027 -0.000036 -0.000046 0.000013

25 26 27

1 C 0.000000 0.000000 0.000000

2 C 0.000000 0.000000 0.000000

3 O 0.000000 0.000000 0.000000

4 O 0.000000 0.000000 0.000000

5 C 0.000000 0.000000 0.000000

6 S 0.000000 0.000000 0.000000

7 C 0.000000 0.000000 0.000000

8 S -0.000005 -0.000023 0.000018

9 S 0.000000 0.000000 -0.000001

10 C 0.000000 0.000001 -0.000008

11 C -0.000018 0.000002 0.000064

12 C 0.000038 0.000083 -0.000119

13 C -0.000036 -0.000070 0.000045

14 H 0.000000 0.000000 0.000000

15 H 0.000000 0.000000 0.000000

16 H 0.000000 0.000000 0.000000

17 H 0.000000 0.000000 0.000000

18 H 0.000000 0.000000 0.000000

19 H -0.000010 -0.000009 0.000030

20 H 0.000005 0.000009 -0.000009

21 H -0.000009 -0.000032 0.000027

22 H 0.000009 0.000012 -0.000036

23 H 0.000041 0.000015 -0.000046

24 H -0.000020 -0.000017 0.000013

25 H 0.000018 0.000030 -0.000039

26 H 0.000030 0.000043 -0.000031

27 H -0.000039 -0.000031 0.000083

Mulliken charges and spin densities:

1 2

1 C 0.427124 0.013133

2 C -0.434541 0.079199

3 O -0.370042 0.012765

4 O -0.506799 0.003914

5 C -0.618398 -0.000709

6 S 0.080938 0.016427

7 C -0.550340 0.525170

8 S 0.126547 0.079715

9 S -0.500053 0.260790

10 C -0.551401 0.008127

11 C -0.418041 -0.000824

12 C -0.395515 -0.000267

13 C -0.641193 0.000193

14 H 0.270948 -0.003156

15 H 0.413446 0.000069

16 H 0.245064 -0.001884

17 H 0.224640 0.001469

18 H 0.225252 0.000306

19 H 0.238534 0.006220

20 H 0.252881 -0.001241

21 H 0.212890 0.000472

22 H 0.213088 0.000093

23 H 0.208316 -0.000063

24 H 0.208303 0.000074

25 H 0.215193 0.000004

26 H 0.211554 0.000013

27 H 0.211606 -0.000008

Sum of Mulliken charges = -1.00000 1.00000

Mulliken charges and spin densities with hydrogens summed into heavy atoms:

1 2

1 C 0.427124 0.013133

2 C -0.163593 0.076043

3 O -0.370042 0.012765

4 O -0.093353 0.003983

5 C 0.076558 -0.000817

6 S 0.080938 0.016427

7 C -0.550340 0.525170

8 S 0.126547 0.079715

9 S -0.500053 0.260790

10 C -0.059986 0.013106

11 C 0.007937 -0.000259

12 C 0.021103 -0.000256

13 C -0.002840 0.000202

Electronic spatial extent (au): <R\*\*2>= 6009.3602

Charge= -1.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 3.6191 Y= -7.5280 Z= 1.6041 Tot= 8.5054

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -111.5196 YY= -127.0313 ZZ= -111.3586

XY= 10.8675 XZ= -8.8347 YZ= 0.6128

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= 5.1169 YY= -10.3948 ZZ= 5.2779

XY= 10.8675 XZ= -8.8347 YZ= 0.6128

Octapole moment (field-independent basis, Debye-Ang\*\*2):

XXX= 16.1924 YYY= -72.0984 ZZZ= -0.8942 XYY= -26.2950

XXY= -63.0109 XXZ= 26.5870 XZZ= -2.9080 YZZ= -12.0063

YYZ= -6.4948 XYZ= -13.7799

Hexadecapole moment (field-independent basis, Debye-Ang\*\*3):

XXXX= -6968.8990 YYYY= -1053.7955 ZZZZ= -451.1402 XXXY= 419.4441

XXXZ= -118.2024 YYYX= 78.3304 YYYZ= 2.6459 ZZZX= -9.1233

ZZZY= -6.4682 XXYY= -1224.2321 XXZZ= -1225.3564 YYZZ= -243.2586

XXYZ= 61.9434 YYXZ= 19.4441 ZZXY= 17.7095

N-N= 1.102306838177D+03 E-N=-6.147376174045D+03 KE= 1.655235388723D+03

Isotropic Fermi Contact Couplings

Atom a.u. MegaHertz Gauss 10(-4) cm-1

1 C(13) 0.00102 1.14451 0.40839 0.38177

2 C(13) 0.04780 53.73170 19.17281 17.92297

3 O(17) 0.00231 -1.40021 -0.49963 -0.46706

4 O(17) 0.00119 -0.72125 -0.25736 -0.24058

5 C(13) -0.00285 -3.20510 -1.14366 -1.06911

6 S(33) 0.08524 29.27853 10.44731 9.76627

7 C(13) 0.07179 80.70801 28.79862 26.92129

8 S(33) 0.00344 1.18143 0.42156 0.39408

9 S(33) 0.00778 2.67387 0.95410 0.89191

10 C(13) 0.00683 7.68085 2.74072 2.56206

11 C(13) -0.00104 -1.17013 -0.41753 -0.39031

12 C(13) 0.00024 0.27532 0.09824 0.09184

13 C(13) 0.00014 0.15230 0.05434 0.05080

14 H(1) -0.00104 -4.65632 -1.66149 -1.55318

15 H(1) -0.00010 -0.44411 -0.15847 -0.14814

16 H(1) 0.00021 0.93701 0.33435 0.31255

17 H(1) 0.00104 4.66481 1.66452 1.55601

18 H(1) 0.00021 0.94133 0.33589 0.31399

19 H(1) 0.00156 6.97903 2.49029 2.32795

20 H(1) 0.00031 1.38627 0.49466 0.46241

21 H(1) -0.00005 -0.23157 -0.08263 -0.07724

22 H(1) 0.00008 0.34811 0.12421 0.11612

23 H(1) 0.00011 0.47546 0.16965 0.15860

24 H(1) 0.00001 0.02577 0.00920 0.00860

25 H(1) 0.00000 -0.01595 -0.00569 -0.00532

26 H(1) 0.00000 -0.00982 -0.00350 -0.00327

27 H(1) 0.00000 -0.00742 -0.00265 -0.00248

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Center ---- Spin Dipole Couplings ----

3XX-RR 3YY-RR 3ZZ-RR

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1 Atom -0.010565 -0.010157 0.020722

2 Atom 0.029587 -0.051967 0.022381

3 Atom -0.026795 -0.015259 0.042054

4 Atom -0.001107 -0.004968 0.006075

5 Atom 0.000384 -0.002417 0.002033

6 Atom 0.035558 0.107406 -0.142964

7 Atom -0.207887 -0.307766 0.515654

8 Atom -0.211672 -0.258618 0.470290

9 Atom -0.112513 -0.531674 0.644187

10 Atom 0.016736 -0.005147 -0.011589

11 Atom 0.002002 -0.001876 -0.000126

12 Atom 0.001736 -0.000958 -0.000778

13 Atom 0.000927 -0.000336 -0.000591

14 Atom 0.002531 0.003237 -0.005768

15 Atom 0.001171 -0.000060 -0.001111

16 Atom -0.001684 -0.003571 0.005255

17 Atom 0.000178 -0.001670 0.001492

18 Atom -0.000269 0.001401 -0.001132

19 Atom 0.006412 -0.003445 -0.002967

20 Atom 0.004381 -0.001452 -0.002930

21 Atom 0.002523 -0.001076 -0.001447

22 Atom 0.001809 -0.000371 -0.001438

23 Atom 0.001613 -0.000818 -0.000795

24 Atom 0.001588 -0.000786 -0.000801

25 Atom 0.000650 -0.000300 -0.000349

26 Atom 0.000697 -0.000291 -0.000406

27 Atom 0.000661 -0.000249 -0.000412

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XY XZ YZ

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1 Atom 0.000618 -0.002054 0.010532

2 Atom -0.005190 -0.078931 0.007682

3 Atom -0.011093 -0.014457 0.035450

4 Atom -0.007013 -0.014486 0.014145

5 Atom 0.002109 -0.003117 -0.002849

6 Atom -0.191834 0.037969 0.042836

7 Atom 0.087058 -0.361209 -0.206626

8 Atom 0.037850 0.175074 -0.011936

9 Atom 0.141063 -0.673607 -0.291737

10 Atom 0.009198 -0.004881 -0.002130

11 Atom -0.001235 0.001069 -0.001035

12 Atom -0.000475 0.000344 -0.000036

13 Atom -0.000527 -0.000003 -0.000005

14 Atom -0.001956 -0.004227 0.003757

15 Atom 0.001773 0.000763 0.000640

16 Atom 0.002003 -0.004676 -0.003587

17 Atom 0.001023 -0.001379 -0.001590

18 Atom 0.001818 -0.001043 -0.003235

19 Atom 0.000114 -0.002321 -0.000951

20 Atom 0.001234 0.002970 0.000766

21 Atom -0.001558 0.000628 -0.000598

22 Atom -0.001910 -0.000834 0.000377

23 Atom -0.000100 -0.000496 -0.000066

24 Atom 0.000005 0.000372 -0.000005

25 Atom -0.000161 -0.000016 -0.000003

26 Atom -0.000396 0.000161 -0.000076

27 Atom -0.000436 -0.000151 0.000064

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Anisotropic Spin Dipole Couplings in Principal Axis System

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Atom a.u. MegaHertz Gauss 10(-4) cm-1 Axes

Baa -0.0139 -1.859 -0.663 -0.620 -0.3497 0.8902 -0.2919

1 C(13) Bbb -0.0102 -1.370 -0.489 -0.457 0.9354 0.3489 -0.0567

Bcc 0.0241 3.229 1.152 1.077 -0.0514 0.2929 0.9548

Baa -0.0547 -7.346 -2.621 -2.450 -0.4938 0.6561 -0.5707

2 C(13) Bbb -0.0508 -6.814 -2.431 -2.273 0.4856 0.7525 0.4449

Bcc 0.1055 14.159 5.052 4.723 0.7214 -0.0574 -0.6902

Baa -0.0351 2.539 0.906 0.847 0.6053 0.7602 -0.2359

3 O(17) Bbb -0.0275 1.986 0.709 0.663 0.7715 -0.4874 0.4090

Bcc 0.0625 -4.526 -1.615 -1.510 -0.1960 0.4296 0.8815

Baa -0.0155 1.124 0.401 0.375 0.3470 -0.6609 0.6654

4 O(17) Bbb -0.0098 0.712 0.254 0.237 0.7824 0.5952 0.1831

Bcc 0.0254 -1.835 -0.655 -0.612 -0.5171 0.4571 0.7236

Baa -0.0039 -0.526 -0.188 -0.176 -0.2126 0.9201 0.3289

5 C(13) Bbb -0.0020 -0.270 -0.096 -0.090 0.8015 -0.0284 0.5973

Bcc 0.0059 0.797 0.284 0.266 -0.5589 -0.3906 0.7315

Baa -0.1908 -7.823 -2.791 -2.610 -0.4865 -0.4228 0.7646

6 S(33) Bbb -0.0760 -3.117 -1.112 -1.040 0.5988 0.4758 0.6442

Bcc 0.2668 10.940 3.904 3.649 -0.6362 0.7713 0.0217

Baa -0.3586 -48.117 -17.169 -16.050 0.7502 -0.6420 0.1582

7 C(13) Bbb -0.3557 -47.734 -17.033 -15.922 0.5455 0.7362 0.4007

Bcc 0.7143 95.851 34.202 31.973 -0.3737 -0.2143 0.9025

Baa -0.2960 -12.135 -4.330 -4.048 -0.6664 0.7275 0.1636

8 S(33) Bbb -0.2166 -8.882 -3.169 -2.963 0.7077 0.6861 -0.1684

Bcc 0.5126 21.017 7.499 7.010 0.2348 -0.0035 0.9720

Baa -0.6022 -24.688 -8.809 -8.235 0.1255 0.9488 0.2899

9 S(33) Bbb -0.5001 -20.506 -7.317 -6.840 0.8610 -0.2493 0.4433

Bcc 1.1023 45.194 16.126 15.075 -0.4929 -0.1940 0.8482

Baa -0.0125 -1.675 -0.598 -0.559 0.1229 0.1315 0.9837

10 C(13) Bbb -0.0085 -1.137 -0.406 -0.379 -0.3553 0.9313 -0.0801

Bcc 0.0210 2.812 1.003 0.938 0.9266 0.3397 -0.1612

Baa -0.0025 -0.333 -0.119 -0.111 0.1775 0.9279 0.3277

11 C(13) Bbb -0.0005 -0.063 -0.022 -0.021 -0.4754 -0.2107 0.8542

Bcc 0.0029 0.395 0.141 0.132 0.8617 -0.3074 0.4037

Baa -0.0010 -0.140 -0.050 -0.047 0.1800 0.9784 -0.1016

12 C(13) Bbb -0.0008 -0.110 -0.039 -0.037 -0.1101 0.1227 0.9863

Bcc 0.0019 0.250 0.089 0.083 0.9775 -0.1664 0.1298

Baa -0.0006 -0.079 -0.028 -0.026 0.0314 0.0841 0.9960

13 C(13) Bbb -0.0005 -0.071 -0.025 -0.024 0.3392 0.9364 -0.0897

Bcc 0.0011 0.150 0.054 0.050 0.9402 -0.3406 -0.0009

Baa -0.0082 -4.392 -1.567 -1.465 0.3151 -0.2465 0.9165

14 H(1) Bbb 0.0009 0.503 0.180 0.168 0.7119 0.7000 -0.0565

Bcc 0.0073 3.889 1.388 1.297 -0.6276 0.6703 0.3961

Baa -0.0014 -0.761 -0.272 -0.254 0.1795 -0.5987 0.7806

15 H(1) Bbb -0.0013 -0.675 -0.241 -0.225 0.5923 -0.5678 -0.5716

Bcc 0.0027 1.436 0.512 0.479 0.7855 0.5649 0.2527

Baa -0.0049 -2.639 -0.942 -0.880 -0.3002 0.9346 0.1910

16 H(1) Bbb -0.0040 -2.138 -0.763 -0.713 0.8510 0.1719 0.4962

Bcc 0.0090 4.777 1.705 1.593 -0.4309 -0.3115 0.8469

Baa -0.0024 -1.290 -0.460 -0.430 -0.2039 0.9299 0.3062

17 H(1) Bbb -0.0007 -0.370 -0.132 -0.123 0.8430 0.0077 0.5378

Bcc 0.0031 1.660 0.592 0.554 -0.4977 -0.3678 0.7855

Baa -0.0034 -1.788 -0.638 -0.596 -0.0663 0.5788 0.8128

18 H(1) Bbb -0.0012 -0.624 -0.223 -0.208 0.9141 -0.2914 0.2820

Bcc 0.0045 2.412 0.861 0.805 0.4000 0.7616 -0.5098

Baa -0.0044 -2.338 -0.834 -0.780 0.1439 0.6960 0.7035

19 H(1) Bbb -0.0026 -1.378 -0.492 -0.460 -0.1826 0.7173 -0.6724

Bcc 0.0070 3.717 1.326 1.240 0.9726 0.0317 -0.2303

Baa -0.0040 -2.147 -0.766 -0.716 -0.3133 -0.1297 0.9407

20 H(1) Bbb -0.0017 -0.903 -0.322 -0.301 -0.2262 0.9723 0.0587

Bcc 0.0057 3.050 1.088 1.017 0.9223 0.1944 0.3340

Baa -0.0020 -1.044 -0.373 -0.348 0.1628 0.7343 0.6590

21 H(1) Bbb -0.0013 -0.684 -0.244 -0.228 -0.3578 -0.5785 0.7330

Bcc 0.0032 1.729 0.617 0.577 0.9195 -0.3552 0.1685

Baa -0.0017 -0.889 -0.317 -0.296 0.3731 0.2946 0.8798

22 H(1) Bbb -0.0014 -0.766 -0.273 -0.255 0.3721 0.8211 -0.4328

Bcc 0.0031 1.655 0.590 0.552 0.8499 -0.4888 -0.1968

Baa -0.0009 -0.506 -0.181 -0.169 0.1792 0.5514 0.8148

23 H(1) Bbb -0.0008 -0.408 -0.146 -0.136 -0.0789 0.8336 -0.5468

Bcc 0.0017 0.915 0.326 0.305 0.9807 -0.0337 -0.1928

Baa -0.0009 -0.458 -0.163 -0.153 -0.1500 0.0831 0.9852

24 H(1) Bbb -0.0008 -0.419 -0.150 -0.140 0.0107 0.9965 -0.0824

Bcc 0.0016 0.877 0.313 0.293 0.9886 0.0018 0.1504

Baa -0.0004 -0.187 -0.067 -0.062 0.0525 0.2278 0.9723

25 H(1) Bbb -0.0003 -0.174 -0.062 -0.058 0.1548 0.9600 -0.2333

Bcc 0.0007 0.361 0.129 0.120 0.9866 -0.1628 -0.0151

Baa -0.0004 -0.240 -0.085 -0.080 0.1394 0.6916 0.7087

26 H(1) Bbb -0.0004 -0.220 -0.078 -0.073 -0.3295 -0.6425 0.6918

Bcc 0.0009 0.459 0.164 0.153 0.9338 -0.3300 0.1383

Baa -0.0004 -0.232 -0.083 -0.077 0.0131 -0.2986 0.9543

27 H(1) Bbb -0.0004 -0.226 -0.081 -0.075 0.3911 0.8799 0.2699

Bcc 0.0009 0.458 0.163 0.153 0.9202 -0.3697 -0.1283

---------------------------------------------------------------------------------

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Sat Aug 17 18:01:48 2019, MaxMem= 1342177280 cpu: 2.2

(Enter /apps/gaussian/g09d01/g09/l9999.exe)

1\1\GINC-K019\FOpt\UB3LYP\6-311G(d)\C8H14O2S3(1-,2)\Z5105842\17-Aug-20

19\0\\#p opt b3lyp/6-311g\* scrf=(solvent=dmso,smd) empiricaldispersion

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-2.8437027431,0.0748156735,0.4745908192\O,-4.911409879,0.3099350471,-0

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3223,-1.9703885424,-0.6693405801\H,-1.3855669146,-0.3651274757,1.98426

54072\H,-3.0181385678,-0.9092606382,2.3860789049\H,-2.0493480931,-1.80

99972225,1.2059042351\H,2.6882652187,0.9992065365,-0.8767881\H,2.74612

6381,0.9518026148,0.8885923344\H,3.7877831746,-1.3438636666,0.77997712

48\H,3.7570142072,-1.2698596078,-0.9757145583\H,5.2502886245,0.7478228

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303,-0.4032501964,-0.1369900922\H,6.3696855126,-1.6156810192,0.7125145

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3.8798097,-7.5633732,3.6835635,9.0564968,-5.1554082,-1.3857442\PG=C01

[X(C8H14O2S3)]\\@

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GETTING A THIMBLE OF WATER FROM A FIRE HYDRANT.

-- PROF. LEN SHAPIRO, NDSU

Job cpu time: 0 days 6 hours 24 minutes 13.7 seconds.

File lengths (MBytes): RWF= 333 Int= 0 D2E= 0 Chk= 13 Scr= 2

Normal termination of Gaussian 09 at Sat Aug 17 18:01:49 2019.