Entering Gaussian System, Link 0=g09

Input=TPPanion.com

Output=TPPanion.log

Initial command:

/home/kira/g09/l1.exe "/home/kira/g09/scratch/Gau-13910.inp" -scrdir="/home/kira/g09/scratch/"

Entering Link 1 = /home/kira/g09/l1.exe PID= 13917.

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340 Quinnipiac St., Bldg. 40, Wallingford CT 06492

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Cite this work as:

Gaussian 09, Revision E.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-G09RevE.01 30-Nov-2015

18-Aug-2019

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

%nprocshared=8

Will use up to 8 processors via shared memory.

%mem=15GB

%chk=TPPanion.chk

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

#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 Sun Aug 18 13:41:10 2019, MaxMem= 2013265920 cpu: 0.4

(Enter /home/kira/g09/l101.exe)

--------

TPPanion

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Symbolic Z-matrix:

Charge = -1 Multiplicity = 2

C 4.21389 -0.42395 0.68324

C 2.88619 -0.11273 1.13348

N 2.11682 0.03992 0.

C 2.88619 -0.11273 -1.13348

C 4.21389 -0.42395 -0.68324

C 2.45221 0.0273 -2.45488

C 1.09152 0.20895 -2.86788

N -0.00037 0.01772 -2.06142

C -1.09097 0.21653 -2.86768

C -0.68714 0.58253 -4.19271

C 0.68992 0.57766 -4.19294

C 2.45221 0.0273 2.45488

C 1.09152 0.20895 2.86788

C 0.68992 0.57766 4.19294

C -0.68714 0.58253 4.19271

C -1.09097 0.21653 2.86768

N -0.00037 0.01772 2.06142

C -2.45285 0.04052 2.45532

C -2.88773 -0.09371 1.13351

C -4.21169 -0.42011 0.68325

C -4.21169 -0.42011 -0.68325

C -2.88773 -0.09371 -1.13351

N -2.12082 0.06983 0.

C -2.45285 0.04052 -2.45532

C 3.48887 -0.01045 -3.51555

C 4.5685 0.8843 -3.50112

C 5.53477 0.84415 -4.50269

C 5.44432 -0.09784 -5.52602

C 4.37599 -0.99501 -5.54798

C 3.40068 -0.94552 -4.55779

C 5.44432 -0.09784 5.52602

C 5.53477 0.84415 4.50269

C 4.5685 0.8843 3.50112

C 3.48887 -0.01045 3.51555

C 3.40068 -0.94552 4.55779

C 4.37599 -0.99501 5.54798

C -3.48841 -0.00504 -3.51618

C -3.39355 -0.94079 -4.55748

C -4.3693 -0.99973 -5.54659

C -5.44502 -0.11138 -5.52488

C -5.54228 0.83128 -4.50279

C -4.57556 0.8808 -3.50213

C -3.48841 -0.00504 3.51618

C -3.39355 -0.94079 4.55748

C -4.3693 -0.99973 5.54659

C -5.44502 -0.11138 5.52488

C -5.54228 0.83128 4.50279

C -4.57556 0.8808 3.50213

H 5.04834 -0.63915 1.33072

H 5.04834 -0.63915 -1.33072

H -1.34144 0.82494 -5.01638

H 1.34552 0.81555 -5.01686

H 1.34552 0.81555 5.01686

H -1.34144 0.82494 5.01638

H -5.04257 -0.64845 1.33081

H -5.04257 -0.64845 -1.33081

H 4.63677 1.62467 -2.71219

H 6.35747 1.55104 -4.48375

H 6.20037 -0.13223 -6.30325

H 4.3022 -1.73448 -6.33834

H 2.57351 -1.64553 -4.57642

H 6.20037 -0.13223 6.30325

H 6.35747 1.55104 4.48375

H 4.63677 1.62467 2.71219

H 2.57351 -1.64553 4.57642

H 4.3022 -1.73448 6.33834

H -2.56119 -1.63456 -4.57565

H -4.29027 -1.73986 -6.33583

H -6.20153 -0.15319 -6.30129

H -6.37076 1.53138 -4.48412

H -4.64945 1.62165 -2.71418

H -2.56119 -1.63456 4.57565

H -4.29027 -1.73986 6.33583

H -6.20153 -0.15319 6.30129

H -6.37076 1.53138 4.48412

H -4.64945 1.62165 2.71418

H 1.11742 0.19455 0.

H -1.12648 0.25294 0.

NAtoms= 78 NQM= 78 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 14 12 12 12 12 14 12 12

AtmWgt= 12.0000000 12.0000000 14.0030740 12.0000000 12.0000000 12.0000000 12.0000000 14.0030740 12.0000000 12.0000000

NucSpn= 0 0 2 0 0 0 0 2 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 2.0440000 0.0000000 0.0000000 0.0000000 0.0000000 2.0440000 0.0000000 0.0000000

NMagM= 0.0000000 0.0000000 0.4037610 0.0000000 0.0000000 0.0000000 0.0000000 0.4037610 0.0000000 0.0000000

AtZNuc= 6.0000000 6.0000000 7.0000000 6.0000000 6.0000000 6.0000000 6.0000000 7.0000000 6.0000000 6.0000000

Atom 11 12 13 14 15 16 17 18 19 20

IAtWgt= 12 12 12 12 12 12 14 12 12 12

AtmWgt= 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 14.0030740 12.0000000 12.0000000 12.0000000

NucSpn= 0 0 0 0 0 0 2 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 2.0440000 0.0000000 0.0000000 0.0000000

NMagM= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.4037610 0.0000000 0.0000000 0.0000000

AtZNuc= 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 7.0000000 6.0000000 6.0000000 6.0000000

Atom 21 22 23 24 25 26 27 28 29 30

IAtWgt= 12 12 14 12 12 12 12 12 12 12

AtmWgt= 12.0000000 12.0000000 14.0030740 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000

NucSpn= 0 0 2 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 2.0440000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NMagM= 0.0000000 0.0000000 0.4037610 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

AtZNuc= 6.0000000 6.0000000 7.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000

Atom 31 32 33 34 35 36 37 38 39 40

IAtWgt= 12 12 12 12 12 12 12 12 12 12

AtmWgt= 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 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 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000

Atom 41 42 43 44 45 46 47 48 49 50

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

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

NucSpn= 0 0 0 0 0 0 0 0 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 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 2.7928460 2.7928460

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

Atom 51 52 53 54 55 56 57 58 59 60

IAtWgt= 1 1 1 1 1 1 1 1 1 1

AtmWgt= 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250

NucSpn= 1 1 1 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= 2.7928460 2.7928460 2.7928460 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 1.0000000 1.0000000 1.0000000

Atom 61 62 63 64 65 66 67 68 69 70

IAtWgt= 1 1 1 1 1 1 1 1 1 1

AtmWgt= 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250

NucSpn= 1 1 1 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= 2.7928460 2.7928460 2.7928460 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 1.0000000 1.0000000 1.0000000

Atom 71 72 73 74 75 76 77 78

IAtWgt= 1 1 1 1 1 1 1 1

AtmWgt= 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250

NucSpn= 1 1 1 1 1 1 1 1

AtZEff= 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

NMagM= 2.7928460 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 1.0000000

Leave Link 101 at Sun Aug 18 13:41:10 2019, MaxMem= 2013265920 cpu: 2.8

(Enter /home/kira/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Initialization pass.

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

! Initial Parameters !

! (Angstroms and Degrees) !

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

! Name Definition Value Derivative Info. !

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

! R1 R(1,2) 1.4361 estimate D2E/DX2 !

! R2 R(1,5) 1.3665 estimate D2E/DX2 !

! R3 R(1,49) 1.0779 estimate D2E/DX2 !

! R4 R(2,3) 1.3784 estimate D2E/DX2 !

! R5 R(2,12) 1.3979 estimate D2E/DX2 !

! R6 R(3,4) 1.3784 estimate D2E/DX2 !

! R7 R(3,77) 1.0113 estimate D2E/DX2 !

! R8 R(4,5) 1.4361 estimate D2E/DX2 !

! R9 R(4,6) 1.3979 estimate D2E/DX2 !

! R10 R(5,50) 1.0779 estimate D2E/DX2 !

! R11 R(6,7) 1.4335 estimate D2E/DX2 !

! R12 R(6,25) 1.4836 estimate D2E/DX2 !

! R13 R(7,8) 1.3708 estimate D2E/DX2 !

! R14 R(7,11) 1.4328 estimate D2E/DX2 !

! R15 R(8,9) 1.3708 estimate D2E/DX2 !

! R16 R(9,10) 1.4327 estimate D2E/DX2 !

! R17 R(9,24) 1.4338 estimate D2E/DX2 !

! R18 R(10,11) 1.3771 estimate D2E/DX2 !

! R19 R(10,51) 1.0795 estimate D2E/DX2 !

! R20 R(11,52) 1.0795 estimate D2E/DX2 !

! R21 R(12,13) 1.4335 estimate D2E/DX2 !

! R22 R(12,34) 1.4836 estimate D2E/DX2 !

! R23 R(13,14) 1.4328 estimate D2E/DX2 !

! R24 R(13,17) 1.3708 estimate D2E/DX2 !

! R25 R(14,15) 1.3771 estimate D2E/DX2 !

! R26 R(14,53) 1.0795 estimate D2E/DX2 !

! R27 R(15,16) 1.4327 estimate D2E/DX2 !

! R28 R(15,54) 1.0795 estimate D2E/DX2 !

! R29 R(16,17) 1.3708 estimate D2E/DX2 !

! R30 R(16,18) 1.4338 estimate D2E/DX2 !

! R31 R(18,19) 1.398 estimate D2E/DX2 !

! R32 R(18,43) 1.4832 estimate D2E/DX2 !

! R33 R(19,20) 1.436 estimate D2E/DX2 !

! R34 R(19,23) 1.3783 estimate D2E/DX2 !

! R35 R(20,21) 1.3665 estimate D2E/DX2 !

! R36 R(20,55) 1.0779 estimate D2E/DX2 !

! R37 R(21,22) 1.436 estimate D2E/DX2 !

! R38 R(21,56) 1.0779 estimate D2E/DX2 !

! R39 R(22,23) 1.3783 estimate D2E/DX2 !

! R40 R(22,24) 1.398 estimate D2E/DX2 !

! R41 R(23,78) 1.0111 estimate D2E/DX2 !

! R42 R(24,37) 1.4832 estimate D2E/DX2 !

! R43 R(25,26) 1.4023 estimate D2E/DX2 !

! R44 R(25,30) 1.403 estimate D2E/DX2 !

! R45 R(26,27) 1.3923 estimate D2E/DX2 !

! R46 R(26,57) 1.0841 estimate D2E/DX2 !

! R47 R(27,28) 1.3938 estimate D2E/DX2 !

! R48 R(27,58) 1.0848 estimate D2E/DX2 !

! R49 R(28,29) 1.3953 estimate D2E/DX2 !

! R50 R(28,59) 1.0848 estimate D2E/DX2 !

! R51 R(29,30) 1.3907 estimate D2E/DX2 !

! R52 R(29,60) 1.0849 estimate D2E/DX2 !

! R53 R(30,61) 1.0838 estimate D2E/DX2 !

! R54 R(31,32) 1.3938 estimate D2E/DX2 !

! R55 R(31,36) 1.3953 estimate D2E/DX2 !

! R56 R(31,62) 1.0848 estimate D2E/DX2 !

! R57 R(32,33) 1.3923 estimate D2E/DX2 !

! R58 R(32,63) 1.0848 estimate D2E/DX2 !

! R59 R(33,34) 1.4023 estimate D2E/DX2 !

! R60 R(33,64) 1.0841 estimate D2E/DX2 !

! R61 R(34,35) 1.403 estimate D2E/DX2 !

! R62 R(35,36) 1.3907 estimate D2E/DX2 !

! R63 R(35,65) 1.0838 estimate D2E/DX2 !

! R64 R(36,66) 1.0849 estimate D2E/DX2 !

! R65 R(37,38) 1.4032 estimate D2E/DX2 !

! R66 R(37,42) 1.4024 estimate D2E/DX2 !

! R67 R(38,39) 1.3906 estimate D2E/DX2 !

! R68 R(38,67) 1.0837 estimate D2E/DX2 !

! R69 R(39,40) 1.3953 estimate D2E/DX2 !

! R70 R(39,68) 1.0849 estimate D2E/DX2 !

! R71 R(40,41) 1.3938 estimate D2E/DX2 !

! R72 R(40,69) 1.0848 estimate D2E/DX2 !

! R73 R(41,42) 1.3922 estimate D2E/DX2 !

! R74 R(41,70) 1.0848 estimate D2E/DX2 !

! R75 R(42,71) 1.0841 estimate D2E/DX2 !

! R76 R(43,44) 1.4032 estimate D2E/DX2 !

! R77 R(43,48) 1.4024 estimate D2E/DX2 !

! R78 R(44,45) 1.3906 estimate D2E/DX2 !

! R79 R(44,72) 1.0837 estimate D2E/DX2 !

! R80 R(45,46) 1.3953 estimate D2E/DX2 !

! R81 R(45,73) 1.0849 estimate D2E/DX2 !

! R82 R(46,47) 1.3938 estimate D2E/DX2 !

! R83 R(46,74) 1.0848 estimate D2E/DX2 !

! R84 R(47,48) 1.3922 estimate D2E/DX2 !

! R85 R(47,75) 1.0848 estimate D2E/DX2 !

! R86 R(48,76) 1.0841 estimate D2E/DX2 !

! A1 A(2,1,5) 108.2715 estimate D2E/DX2 !

! A2 A(2,1,49) 124.796 estimate D2E/DX2 !

! A3 A(5,1,49) 126.9195 estimate D2E/DX2 !

! A4 A(1,2,3) 106.3927 estimate D2E/DX2 !

! A5 A(1,2,12) 127.2364 estimate D2E/DX2 !

! A6 A(3,2,12) 126.3663 estimate D2E/DX2 !

! A7 A(2,3,4) 110.6336 estimate D2E/DX2 !

! A8 A(2,3,77) 124.6476 estimate D2E/DX2 !

! A9 A(4,3,77) 124.6476 estimate D2E/DX2 !

! A10 A(3,4,5) 106.3927 estimate D2E/DX2 !

! A11 A(3,4,6) 126.3663 estimate D2E/DX2 !

! A12 A(5,4,6) 127.2364 estimate D2E/DX2 !

! A13 A(1,5,4) 108.2715 estimate D2E/DX2 !

! A14 A(1,5,50) 126.9195 estimate D2E/DX2 !

! A15 A(4,5,50) 124.796 estimate D2E/DX2 !

! A16 A(4,6,7) 125.4305 estimate D2E/DX2 !

! A17 A(4,6,25) 117.1505 estimate D2E/DX2 !

! A18 A(7,6,25) 117.4186 estimate D2E/DX2 !

! A19 A(6,7,8) 124.6717 estimate D2E/DX2 !

! A20 A(6,7,11) 124.4077 estimate D2E/DX2 !

! A21 A(8,7,11) 110.8974 estimate D2E/DX2 !

! A22 A(7,8,9) 105.5135 estimate D2E/DX2 !

! A23 A(8,9,10) 110.9013 estimate D2E/DX2 !

! A24 A(8,9,24) 124.6634 estimate D2E/DX2 !

! A25 A(10,9,24) 124.4067 estimate D2E/DX2 !

! A26 A(9,10,11) 106.3263 estimate D2E/DX2 !

! A27 A(9,10,51) 126.3118 estimate D2E/DX2 !

! A28 A(11,10,51) 127.3573 estimate D2E/DX2 !

! A29 A(7,11,10) 106.3224 estimate D2E/DX2 !

! A30 A(7,11,52) 126.3231 estimate D2E/DX2 !

! A31 A(10,11,52) 127.3497 estimate D2E/DX2 !

! A32 A(2,12,13) 125.4305 estimate D2E/DX2 !

! A33 A(2,12,34) 117.1505 estimate D2E/DX2 !

! A34 A(13,12,34) 117.4186 estimate D2E/DX2 !

! A35 A(12,13,14) 124.4077 estimate D2E/DX2 !

! A36 A(12,13,17) 124.6717 estimate D2E/DX2 !

! A37 A(14,13,17) 110.8974 estimate D2E/DX2 !

! A38 A(13,14,15) 106.3224 estimate D2E/DX2 !

! A39 A(13,14,53) 126.3231 estimate D2E/DX2 !

! A40 A(15,14,53) 127.3497 estimate D2E/DX2 !

! A41 A(14,15,16) 106.3263 estimate D2E/DX2 !

! A42 A(14,15,54) 127.3573 estimate D2E/DX2 !

! A43 A(16,15,54) 126.3118 estimate D2E/DX2 !

! A44 A(15,16,17) 110.9013 estimate D2E/DX2 !

! A45 A(15,16,18) 124.4067 estimate D2E/DX2 !

! A46 A(17,16,18) 124.6634 estimate D2E/DX2 !

! A47 A(13,17,16) 105.5135 estimate D2E/DX2 !

! A48 A(16,18,19) 125.3941 estimate D2E/DX2 !

! A49 A(16,18,43) 117.4673 estimate D2E/DX2 !

! A50 A(19,18,43) 117.1386 estimate D2E/DX2 !

! A51 A(18,19,20) 127.2358 estimate D2E/DX2 !

! A52 A(18,19,23) 126.3776 estimate D2E/DX2 !

! A53 A(20,19,23) 106.3861 estimate D2E/DX2 !

! A54 A(19,20,21) 108.2732 estimate D2E/DX2 !

! A55 A(19,20,55) 124.7833 estimate D2E/DX2 !

! A56 A(21,20,55) 126.9249 estimate D2E/DX2 !

! A57 A(20,21,22) 108.2732 estimate D2E/DX2 !

! A58 A(20,21,56) 126.9249 estimate D2E/DX2 !

! A59 A(22,21,56) 124.7833 estimate D2E/DX2 !

! A60 A(21,22,23) 106.3861 estimate D2E/DX2 !

! A61 A(21,22,24) 127.2358 estimate D2E/DX2 !

! A62 A(23,22,24) 126.3776 estimate D2E/DX2 !

! A63 A(19,23,22) 110.6492 estimate D2E/DX2 !

! A64 A(19,23,78) 124.6599 estimate D2E/DX2 !

! A65 A(22,23,78) 124.6599 estimate D2E/DX2 !

! A66 A(9,24,22) 125.3941 estimate D2E/DX2 !

! A67 A(9,24,37) 117.4673 estimate D2E/DX2 !

! A68 A(22,24,37) 117.1386 estimate D2E/DX2 !

! A69 A(6,25,26) 120.9556 estimate D2E/DX2 !

! A70 A(6,25,30) 120.2734 estimate D2E/DX2 !

! A71 A(26,25,30) 118.7706 estimate D2E/DX2 !

! A72 A(25,26,27) 120.5658 estimate D2E/DX2 !

! A73 A(25,26,57) 119.4551 estimate D2E/DX2 !

! A74 A(27,26,57) 119.9681 estimate D2E/DX2 !

! A75 A(26,27,28) 120.1732 estimate D2E/DX2 !

! A76 A(26,27,58) 119.6674 estimate D2E/DX2 !

! A77 A(28,27,58) 120.1593 estimate D2E/DX2 !

! A78 A(27,28,29) 119.7233 estimate D2E/DX2 !

! A79 A(27,28,59) 120.1461 estimate D2E/DX2 !

! A80 A(29,28,59) 120.1305 estimate D2E/DX2 !

! A81 A(28,29,30) 120.1912 estimate D2E/DX2 !

! A82 A(28,29,60) 120.1218 estimate D2E/DX2 !

! A83 A(30,29,60) 119.687 estimate D2E/DX2 !

! A84 A(25,30,29) 120.5668 estimate D2E/DX2 !

! A85 A(25,30,61) 119.4217 estimate D2E/DX2 !

! A86 A(29,30,61) 120.0012 estimate D2E/DX2 !

! A87 A(32,31,36) 119.7233 estimate D2E/DX2 !

! A88 A(32,31,62) 120.1461 estimate D2E/DX2 !

! A89 A(36,31,62) 120.1305 estimate D2E/DX2 !

! A90 A(31,32,33) 120.1732 estimate D2E/DX2 !

! A91 A(31,32,63) 120.1593 estimate D2E/DX2 !

! A92 A(33,32,63) 119.6674 estimate D2E/DX2 !

! A93 A(32,33,34) 120.5658 estimate D2E/DX2 !

! A94 A(32,33,64) 119.9681 estimate D2E/DX2 !

! A95 A(34,33,64) 119.4551 estimate D2E/DX2 !

! A96 A(12,34,33) 120.9556 estimate D2E/DX2 !

! A97 A(12,34,35) 120.2734 estimate D2E/DX2 !

! A98 A(33,34,35) 118.7706 estimate D2E/DX2 !

! A99 A(34,35,36) 120.5668 estimate D2E/DX2 !

! A100 A(34,35,65) 119.4217 estimate D2E/DX2 !

! A101 A(36,35,65) 120.0012 estimate D2E/DX2 !

! A102 A(31,36,35) 120.1912 estimate D2E/DX2 !

! A103 A(31,36,66) 120.1218 estimate D2E/DX2 !

! A104 A(35,36,66) 119.687 estimate D2E/DX2 !

! A105 A(24,37,38) 120.2696 estimate D2E/DX2 !

! A106 A(24,37,42) 120.9749 estimate D2E/DX2 !

! A107 A(38,37,42) 118.7555 estimate D2E/DX2 !

! A108 A(37,38,39) 120.5741 estimate D2E/DX2 !

! A109 A(37,38,67) 119.4244 estimate D2E/DX2 !

! A110 A(39,38,67) 119.9902 estimate D2E/DX2 !

! A111 A(38,39,40) 120.192 estimate D2E/DX2 !

! A112 A(38,39,68) 119.6856 estimate D2E/DX2 !

! A113 A(40,39,68) 120.1224 estimate D2E/DX2 !

! A114 A(39,40,41) 119.7231 estimate D2E/DX2 !

! A115 A(39,40,69) 120.13 estimate D2E/DX2 !

! A116 A(41,40,69) 120.1468 estimate D2E/DX2 !

! A117 A(40,41,42) 120.1757 estimate D2E/DX2 !

! A118 A(40,41,70) 120.1573 estimate D2E/DX2 !

! A119 A(42,41,70) 119.6669 estimate D2E/DX2 !

! A120 A(37,42,41) 120.5705 estimate D2E/DX2 !

! A121 A(37,42,71) 119.4586 estimate D2E/DX2 !

! A122 A(41,42,71) 119.9599 estimate D2E/DX2 !

! A123 A(18,43,44) 120.2696 estimate D2E/DX2 !

! A124 A(18,43,48) 120.9749 estimate D2E/DX2 !

! A125 A(44,43,48) 118.7555 estimate D2E/DX2 !

! A126 A(43,44,45) 120.5741 estimate D2E/DX2 !

! A127 A(43,44,72) 119.4244 estimate D2E/DX2 !

! A128 A(45,44,72) 119.9902 estimate D2E/DX2 !

! A129 A(44,45,46) 120.192 estimate D2E/DX2 !

! A130 A(44,45,73) 119.6856 estimate D2E/DX2 !

! A131 A(46,45,73) 120.1224 estimate D2E/DX2 !

! A132 A(45,46,47) 119.7231 estimate D2E/DX2 !

! A133 A(45,46,74) 120.13 estimate D2E/DX2 !

! A134 A(47,46,74) 120.1468 estimate D2E/DX2 !

! A135 A(46,47,48) 120.1757 estimate D2E/DX2 !

! A136 A(46,47,75) 120.1573 estimate D2E/DX2 !

! A137 A(48,47,75) 119.6669 estimate D2E/DX2 !

! A138 A(43,48,47) 120.5705 estimate D2E/DX2 !

! A139 A(43,48,76) 119.4586 estimate D2E/DX2 !

! A140 A(47,48,76) 119.9599 estimate D2E/DX2 !

! D1 D(5,1,2,3) 1.1683 estimate D2E/DX2 !

! D2 D(5,1,2,12) -178.0794 estimate D2E/DX2 !

! D3 D(49,1,2,3) -177.5969 estimate D2E/DX2 !

! D4 D(49,1,2,12) 3.1555 estimate D2E/DX2 !

! D5 D(2,1,5,4) 0.0 estimate D2E/DX2 !

! D6 D(2,1,5,50) -178.7316 estimate D2E/DX2 !

! D7 D(49,1,5,4) 178.7316 estimate D2E/DX2 !

! D8 D(49,1,5,50) 0.0 estimate D2E/DX2 !

! D9 D(1,2,3,4) -1.9498 estimate D2E/DX2 !

! D10 D(1,2,3,77) 175.0996 estimate D2E/DX2 !

! D11 D(12,2,3,4) 177.3064 estimate D2E/DX2 !

! D12 D(12,2,3,77) -5.6442 estimate D2E/DX2 !

! D13 D(1,2,12,13) -173.4918 estimate D2E/DX2 !

! D14 D(1,2,12,34) 6.7543 estimate D2E/DX2 !

! D15 D(3,2,12,13) 7.4045 estimate D2E/DX2 !

! D16 D(3,2,12,34) -172.3494 estimate D2E/DX2 !

! D17 D(2,3,4,5) 1.9498 estimate D2E/DX2 !

! D18 D(2,3,4,6) -177.3064 estimate D2E/DX2 !

! D19 D(77,3,4,5) -175.0996 estimate D2E/DX2 !

! D20 D(77,3,4,6) 5.6442 estimate D2E/DX2 !

! D21 D(3,4,5,1) -1.1683 estimate D2E/DX2 !

! D22 D(3,4,5,50) 177.5969 estimate D2E/DX2 !

! D23 D(6,4,5,1) 178.0794 estimate D2E/DX2 !

! D24 D(6,4,5,50) -3.1555 estimate D2E/DX2 !

! D25 D(3,4,6,7) -7.4045 estimate D2E/DX2 !

! D26 D(3,4,6,25) 172.3494 estimate D2E/DX2 !

! D27 D(5,4,6,7) 173.4918 estimate D2E/DX2 !

! D28 D(5,4,6,25) -6.7543 estimate D2E/DX2 !

! D29 D(4,6,7,8) -13.1373 estimate D2E/DX2 !

! D30 D(4,6,7,11) 168.7776 estimate D2E/DX2 !

! D31 D(25,6,7,8) 167.1094 estimate D2E/DX2 !

! D32 D(25,6,7,11) -10.9757 estimate D2E/DX2 !

! D33 D(4,6,25,26) -56.6453 estimate D2E/DX2 !

! D34 D(4,6,25,30) 123.5701 estimate D2E/DX2 !

! D35 D(7,6,25,26) 123.1288 estimate D2E/DX2 !

! D36 D(7,6,25,30) -56.6558 estimate D2E/DX2 !

! D37 D(6,7,8,9) -176.3602 estimate D2E/DX2 !

! D38 D(11,7,8,9) 1.9487 estimate D2E/DX2 !

! D39 D(6,7,11,10) 177.0905 estimate D2E/DX2 !

! D40 D(6,7,11,52) -3.6631 estimate D2E/DX2 !

! D41 D(8,7,11,10) -1.2239 estimate D2E/DX2 !

! D42 D(8,7,11,52) 178.0226 estimate D2E/DX2 !

! D43 D(7,8,9,10) -1.9537 estimate D2E/DX2 !

! D44 D(7,8,9,24) 176.1703 estimate D2E/DX2 !

! D45 D(8,9,10,11) 1.2368 estimate D2E/DX2 !

! D46 D(8,9,10,51) -178.0238 estimate D2E/DX2 !

! D47 D(24,9,10,11) -176.8929 estimate D2E/DX2 !

! D48 D(24,9,10,51) 3.8465 estimate D2E/DX2 !

! D49 D(8,9,24,22) 13.4958 estimate D2E/DX2 !

! D50 D(8,9,24,37) -166.4252 estimate D2E/DX2 !

! D51 D(10,9,24,22) -168.6285 estimate D2E/DX2 !

! D52 D(10,9,24,37) 11.4504 estimate D2E/DX2 !

! D53 D(9,10,11,7) -0.0075 estimate D2E/DX2 !

! D54 D(9,10,11,52) -179.2437 estimate D2E/DX2 !

! D55 D(51,10,11,7) 179.2429 estimate D2E/DX2 !

! D56 D(51,10,11,52) 0.0067 estimate D2E/DX2 !

! D57 D(2,12,13,14) -168.7776 estimate D2E/DX2 !

! D58 D(2,12,13,17) 13.1373 estimate D2E/DX2 !

! D59 D(34,12,13,14) 10.9757 estimate D2E/DX2 !

! D60 D(34,12,13,17) -167.1094 estimate D2E/DX2 !

! D61 D(2,12,34,33) 56.6453 estimate D2E/DX2 !

! D62 D(2,12,34,35) -123.5701 estimate D2E/DX2 !

! D63 D(13,12,34,33) -123.1288 estimate D2E/DX2 !

! D64 D(13,12,34,35) 56.6558 estimate D2E/DX2 !

! D65 D(12,13,14,15) -177.0905 estimate D2E/DX2 !

! D66 D(12,13,14,53) 3.6631 estimate D2E/DX2 !

! D67 D(17,13,14,15) 1.2239 estimate D2E/DX2 !

! D68 D(17,13,14,53) -178.0226 estimate D2E/DX2 !

! D69 D(12,13,17,16) 176.3602 estimate D2E/DX2 !

! D70 D(14,13,17,16) -1.9487 estimate D2E/DX2 !

! D71 D(13,14,15,16) 0.0075 estimate D2E/DX2 !

! D72 D(13,14,15,54) -179.2429 estimate D2E/DX2 !

! D73 D(53,14,15,16) 179.2437 estimate D2E/DX2 !

! D74 D(53,14,15,54) -0.0067 estimate D2E/DX2 !

! D75 D(14,15,16,17) -1.2368 estimate D2E/DX2 !

! D76 D(14,15,16,18) 176.8929 estimate D2E/DX2 !

! D77 D(54,15,16,17) 178.0238 estimate D2E/DX2 !

! D78 D(54,15,16,18) -3.8465 estimate D2E/DX2 !

! D79 D(15,16,17,13) 1.9537 estimate D2E/DX2 !

! D80 D(18,16,17,13) -176.1703 estimate D2E/DX2 !

! D81 D(15,16,18,19) 168.6285 estimate D2E/DX2 !

! D82 D(15,16,18,43) -11.4504 estimate D2E/DX2 !

! D83 D(17,16,18,19) -13.4958 estimate D2E/DX2 !

! D84 D(17,16,18,43) 166.4252 estimate D2E/DX2 !

! D85 D(16,18,19,20) 172.4194 estimate D2E/DX2 !

! D86 D(16,18,19,23) -7.9104 estimate D2E/DX2 !

! D87 D(43,18,19,20) -7.502 estimate D2E/DX2 !

! D88 D(43,18,19,23) 172.1683 estimate D2E/DX2 !

! D89 D(16,18,43,44) -56.0216 estimate D2E/DX2 !

! D90 D(16,18,43,48) 123.8973 estimate D2E/DX2 !

! D91 D(19,18,43,44) 123.9061 estimate D2E/DX2 !

! D92 D(19,18,43,48) -56.175 estimate D2E/DX2 !

! D93 D(18,19,20,21) 178.6494 estimate D2E/DX2 !

! D94 D(18,19,20,55) -2.8279 estimate D2E/DX2 !

! D95 D(23,19,20,21) -1.0738 estimate D2E/DX2 !

! D96 D(23,19,20,55) 177.4488 estimate D2E/DX2 !

! D97 D(18,19,23,22) -177.9338 estimate D2E/DX2 !

! D98 D(18,19,23,78) 4.0157 estimate D2E/DX2 !

! D99 D(20,19,23,22) 1.7925 estimate D2E/DX2 !

! D100 D(20,19,23,78) -176.258 estimate D2E/DX2 !

! D101 D(19,20,21,22) 0.0 estimate D2E/DX2 !

! D102 D(19,20,21,56) 178.4822 estimate D2E/DX2 !

! D103 D(55,20,21,22) -178.4822 estimate D2E/DX2 !

! D104 D(55,20,21,56) 0.0 estimate D2E/DX2 !

! D105 D(20,21,22,23) 1.0738 estimate D2E/DX2 !

! D106 D(20,21,22,24) -178.6494 estimate D2E/DX2 !

! D107 D(56,21,22,23) -177.4488 estimate D2E/DX2 !

! D108 D(56,21,22,24) 2.8279 estimate D2E/DX2 !

! D109 D(21,22,23,19) -1.7925 estimate D2E/DX2 !

! D110 D(21,22,23,78) 176.258 estimate D2E/DX2 !

! D111 D(24,22,23,19) 177.9338 estimate D2E/DX2 !

! D112 D(24,22,23,78) -4.0157 estimate D2E/DX2 !

! D113 D(21,22,24,9) -172.4194 estimate D2E/DX2 !

! D114 D(21,22,24,37) 7.502 estimate D2E/DX2 !

! D115 D(23,22,24,9) 7.9104 estimate D2E/DX2 !

! D116 D(23,22,24,37) -172.1683 estimate D2E/DX2 !

! D117 D(9,24,37,38) 56.0216 estimate D2E/DX2 !

! D118 D(9,24,37,42) -123.8973 estimate D2E/DX2 !

! D119 D(22,24,37,38) -123.9061 estimate D2E/DX2 !

! D120 D(22,24,37,42) 56.175 estimate D2E/DX2 !

! D121 D(6,25,26,27) -179.8187 estimate D2E/DX2 !

! D122 D(6,25,26,57) -1.0274 estimate D2E/DX2 !

! D123 D(30,25,26,27) -0.031 estimate D2E/DX2 !

! D124 D(30,25,26,57) 178.7604 estimate D2E/DX2 !

! D125 D(6,25,30,29) -179.3642 estimate D2E/DX2 !

! D126 D(6,25,30,61) -0.5353 estimate D2E/DX2 !

! D127 D(26,25,30,29) 0.8465 estimate D2E/DX2 !

! D128 D(26,25,30,61) 179.6755 estimate D2E/DX2 !

! D129 D(25,26,27,28) -0.6117 estimate D2E/DX2 !

! D130 D(25,26,27,58) 179.2682 estimate D2E/DX2 !

! D131 D(57,26,27,28) -179.3969 estimate D2E/DX2 !

! D132 D(57,26,27,58) 0.483 estimate D2E/DX2 !

! D133 D(26,27,28,29) 0.4431 estimate D2E/DX2 !

! D134 D(26,27,28,59) -179.6694 estimate D2E/DX2 !

! D135 D(58,27,28,29) -179.4362 estimate D2E/DX2 !

! D136 D(58,27,28,59) 0.4513 estimate D2E/DX2 !

! D137 D(27,28,29,30) 0.37 estimate D2E/DX2 !

! D138 D(27,28,29,60) -179.6572 estimate D2E/DX2 !

! D139 D(59,28,29,30) -179.5175 estimate D2E/DX2 !

! D140 D(59,28,29,60) 0.4553 estimate D2E/DX2 !

! D141 D(28,29,30,25) -1.022 estimate D2E/DX2 !

! D142 D(28,29,30,61) -179.8441 estimate D2E/DX2 !

! D143 D(60,29,30,25) 179.0051 estimate D2E/DX2 !

! D144 D(60,29,30,61) 0.183 estimate D2E/DX2 !

! D145 D(36,31,32,33) -0.4431 estimate D2E/DX2 !

! D146 D(36,31,32,63) 179.4362 estimate D2E/DX2 !

! D147 D(62,31,32,33) 179.6694 estimate D2E/DX2 !

! D148 D(62,31,32,63) -0.4513 estimate D2E/DX2 !

! D149 D(32,31,36,35) -0.37 estimate D2E/DX2 !

! D150 D(32,31,36,66) 179.6572 estimate D2E/DX2 !

! D151 D(62,31,36,35) 179.5175 estimate D2E/DX2 !

! D152 D(62,31,36,66) -0.4553 estimate D2E/DX2 !

! D153 D(31,32,33,34) 0.6117 estimate D2E/DX2 !

! D154 D(31,32,33,64) 179.3969 estimate D2E/DX2 !

! D155 D(63,32,33,34) -179.2682 estimate D2E/DX2 !

! D156 D(63,32,33,64) -0.483 estimate D2E/DX2 !

! D157 D(32,33,34,12) 179.8187 estimate D2E/DX2 !

! D158 D(32,33,34,35) 0.031 estimate D2E/DX2 !

! D159 D(64,33,34,12) 1.0274 estimate D2E/DX2 !

! D160 D(64,33,34,35) -178.7604 estimate D2E/DX2 !

! D161 D(12,34,35,36) 179.3642 estimate D2E/DX2 !

! D162 D(12,34,35,65) 0.5353 estimate D2E/DX2 !

! D163 D(33,34,35,36) -0.8465 estimate D2E/DX2 !

! D164 D(33,34,35,65) -179.6755 estimate D2E/DX2 !

! D165 D(34,35,36,31) 1.022 estimate D2E/DX2 !

! D166 D(34,35,36,66) -179.0051 estimate D2E/DX2 !

! D167 D(65,35,36,31) 179.8441 estimate D2E/DX2 !

! D168 D(65,35,36,66) -0.183 estimate D2E/DX2 !

! D169 D(24,37,38,39) 179.2256 estimate D2E/DX2 !

! D170 D(24,37,38,67) 0.4541 estimate D2E/DX2 !

! D171 D(42,37,38,39) -0.8537 estimate D2E/DX2 !

! D172 D(42,37,38,67) -179.6252 estimate D2E/DX2 !

! D173 D(24,37,42,41) 179.9519 estimate D2E/DX2 !

! D174 D(24,37,42,71) 1.1565 estimate D2E/DX2 !

! D175 D(38,37,42,41) 0.0318 estimate D2E/DX2 !

! D176 D(38,37,42,71) -178.7636 estimate D2E/DX2 !

! D177 D(37,38,39,40) 1.0293 estimate D2E/DX2 !

! D178 D(37,38,39,68) -178.9826 estimate D2E/DX2 !

! D179 D(67,38,39,40) 179.7939 estimate D2E/DX2 !

! D180 D(67,38,39,68) -0.218 estimate D2E/DX2 !

! D181 D(38,39,40,41) -0.371 estimate D2E/DX2 !

! D182 D(38,39,40,69) 179.5233 estimate D2E/DX2 !

! D183 D(68,39,40,41) 179.641 estimate D2E/DX2 !

! D184 D(68,39,40,69) -0.4648 estimate D2E/DX2 !

! D185 D(39,40,41,42) -0.4484 estimate D2E/DX2 !

! D186 D(39,40,41,70) 179.4328 estimate D2E/DX2 !

! D187 D(69,40,41,42) 179.6574 estimate D2E/DX2 !

! D188 D(69,40,41,70) -0.4614 estimate D2E/DX2 !

! D189 D(40,41,42,37) 0.617 estimate D2E/DX2 !

! D190 D(40,41,42,71) 179.4063 estimate D2E/DX2 !

! D191 D(70,41,42,37) -179.2648 estimate D2E/DX2 !

! D192 D(70,41,42,71) -0.4755 estimate D2E/DX2 !

! D193 D(18,43,44,45) -179.2256 estimate D2E/DX2 !

! D194 D(18,43,44,72) -0.4541 estimate D2E/DX2 !

! D195 D(48,43,44,45) 0.8537 estimate D2E/DX2 !

! D196 D(48,43,44,72) 179.6252 estimate D2E/DX2 !

! D197 D(18,43,48,47) -179.9519 estimate D2E/DX2 !

! D198 D(18,43,48,76) -1.1565 estimate D2E/DX2 !

! D199 D(44,43,48,47) -0.0318 estimate D2E/DX2 !

! D200 D(44,43,48,76) 178.7636 estimate D2E/DX2 !

! D201 D(43,44,45,46) -1.0293 estimate D2E/DX2 !

! D202 D(43,44,45,73) 178.9826 estimate D2E/DX2 !

! D203 D(72,44,45,46) -179.7939 estimate D2E/DX2 !

! D204 D(72,44,45,73) 0.218 estimate D2E/DX2 !

! D205 D(44,45,46,47) 0.371 estimate D2E/DX2 !

! D206 D(44,45,46,74) -179.5233 estimate D2E/DX2 !

! D207 D(73,45,46,47) -179.641 estimate D2E/DX2 !

! D208 D(73,45,46,74) 0.4648 estimate D2E/DX2 !

! D209 D(45,46,47,48) 0.4484 estimate D2E/DX2 !

! D210 D(45,46,47,75) -179.4328 estimate D2E/DX2 !

! D211 D(74,46,47,48) -179.6574 estimate D2E/DX2 !

! D212 D(74,46,47,75) 0.4614 estimate D2E/DX2 !

! D213 D(46,47,48,43) -0.617 estimate D2E/DX2 !

! D214 D(46,47,48,76) -179.4063 estimate D2E/DX2 !

! D215 D(75,47,48,43) 179.2648 estimate D2E/DX2 !

! D216 D(75,47,48,76) 0.4755 estimate D2E/DX2 !

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

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

Number of steps in this run= 452 maximum allowed number of steps= 468.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Aug 18 13:41:10 2019, MaxMem= 2013265920 cpu: 0.1

(Enter /home/kira/g09/l202.exe)

Stoichiometry C44H30N4(1-,2)

Framework group CS[SG(H2N2),X(C44H28N2)]

Deg. of freedom 116

Full point group CS NOp 2

Largest Abelian subgroup CS NOp 2

Largest concise Abelian subgroup CS NOp 2

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.423954 -4.213891 0.683236

2 6 0 -0.112734 -2.886189 1.133480

3 7 0 0.039918 -2.116820 0.000000

4 6 0 -0.112734 -2.886189 -1.133480

5 6 0 -0.423954 -4.213891 -0.683236

6 6 0 0.027303 -2.452207 -2.454876

7 6 0 0.208949 -1.091519 -2.867880

8 7 0 0.017718 0.000367 -2.061423

9 6 0 0.216526 1.090968 -2.867677

10 6 0 0.582527 0.687135 -4.192709

11 6 0 0.577656 -0.689918 -4.192935

12 6 0 0.027303 -2.452207 2.454876

13 6 0 0.208949 -1.091519 2.867880

14 6 0 0.577656 -0.689918 4.192935

15 6 0 0.582527 0.687135 4.192709

16 6 0 0.216526 1.090968 2.867677

17 7 0 0.017718 0.000367 2.061423

18 6 0 0.040515 2.452854 2.455321

19 6 0 -0.093714 2.887734 1.133508

20 6 0 -0.420105 4.211686 0.683250

21 6 0 -0.420105 4.211686 -0.683250

22 6 0 -0.093714 2.887734 -1.133508

23 7 0 0.069828 2.120819 -0.000000

24 6 0 0.040515 2.452854 -2.455321

25 6 0 -0.010453 -3.488874 -3.515546

26 6 0 0.884303 -4.568500 -3.501119

27 6 0 0.844149 -5.534768 -4.502692

28 6 0 -0.097843 -5.444323 -5.526017

29 6 0 -0.995008 -4.375987 -5.547976

30 6 0 -0.945522 -3.400677 -4.557787

31 6 0 -0.097843 -5.444323 5.526017

32 6 0 0.844149 -5.534768 4.502692

33 6 0 0.884303 -4.568500 3.501119

34 6 0 -0.010453 -3.488874 3.515546

35 6 0 -0.945522 -3.400677 4.557787

36 6 0 -0.995008 -4.375987 5.547976

37 6 0 -0.005043 3.488412 -3.516184

38 6 0 -0.940791 3.393551 -4.557483

39 6 0 -0.999731 4.369301 -5.546591

40 6 0 -0.111382 5.445016 -5.524878

41 6 0 0.831275 5.542283 -4.502786

42 6 0 0.880798 4.575556 -3.502133

43 6 0 -0.005043 3.488412 3.516184

44 6 0 -0.940791 3.393551 4.557483

45 6 0 -0.999731 4.369301 5.546591

46 6 0 -0.111382 5.445016 5.524878

47 6 0 0.831275 5.542283 4.502786

48 6 0 0.880798 4.575556 3.502133

49 1 0 -0.639146 -5.048341 1.330716

50 1 0 -0.639146 -5.048341 -1.330716

51 1 0 0.824935 1.341435 -5.016381

52 1 0 0.815547 -1.345523 -5.016864

53 1 0 0.815547 -1.345523 5.016864

54 1 0 0.824935 1.341435 5.016381

55 1 0 -0.648449 5.042574 1.330814

56 1 0 -0.648449 5.042574 -1.330814

57 1 0 1.624673 -4.636766 -2.712187

58 1 0 1.551040 -6.357470 -4.483753

59 1 0 -0.132226 -6.200370 -6.303252

60 1 0 -1.734479 -4.302196 -6.338340

61 1 0 -1.645533 -2.573509 -4.576424

62 1 0 -0.132226 -6.200370 6.303252

63 1 0 1.551040 -6.357470 4.483753

64 1 0 1.624673 -4.636766 2.712187

65 1 0 -1.645533 -2.573509 4.576424

66 1 0 -1.734479 -4.302196 6.338340

67 1 0 -1.634564 2.561186 -4.575648

68 1 0 -1.739856 4.290269 -6.335831

69 1 0 -0.153189 6.201531 -6.301287

70 1 0 1.531384 6.370760 -4.484118

71 1 0 1.621653 4.649449 -2.714182

72 1 0 -1.634564 2.561186 4.575648

73 1 0 -1.739856 4.290269 6.335831

74 1 0 -0.153189 6.201531 6.301287

75 1 0 1.531384 6.370760 4.484118

76 1 0 1.621653 4.649449 2.714182

77 1 0 0.194551 -1.117420 0.000000

78 1 0 0.252939 1.126484 -0.000000

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

Rotational constants (GHZ): 0.0590611 0.0581645 0.0301342

Leave Link 202 at Sun Aug 18 13:41:10 2019, MaxMem= 2013265920 cpu: 0.0

(Enter /home/kira/g09/l301.exe)

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

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

There are 513 symmetry adapted cartesian basis functions of A' symmetry.

There are 489 symmetry adapted cartesian basis functions of A" symmetry.

There are 488 symmetry adapted basis functions of A' symmetry.

There are 466 symmetry adapted basis functions of A" symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 161 beta electrons

nuclear repulsion energy 5359.8186566968 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= 78 NActive= 78 NUniq= 41 SFac= 3.62D+00 NAtFMM= 60 NAOKFM=T 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= -0.2123119103 Hartrees.

Nuclear repulsion after empirical dispersion term = 5359.6063447864 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= 78.

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

Smoothing algorithm: York/Karplus (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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5742

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.29D-11

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 277

GePol: Fraction of low-weight points (<1% of avg) = 4.82%

GePol: Cavity surface area = 611.256 Ang\*\*2

GePol: Cavity volume = 627.808 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0021258577 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5359.6042189287 Hartrees.

Leave Link 301 at Sun Aug 18 13:41:10 2019, MaxMem= 2013265920 cpu: 1.0

(Enter /home/kira/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.

One-electron integral symmetry used in STVInt

NBasis= 954 RedAO= T EigKep= 9.16D-05 NBF= 488 466

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 488 466

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= 940 940 940 940 940 MxSgAt= 78 MxSgA2= 78.

Leave Link 302 at Sun Aug 18 13:41:12 2019, MaxMem= 2013265920 cpu: 10.8

(Enter /home/kira/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sun Aug 18 13:41:12 2019, MaxMem= 2013265920 cpu: 1.3

(Enter /home/kira/g09/l401.exe)

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2000

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= -1914.57967762745

JPrj=0 DoOrth=F DoCkMO=F.

Initial guess orbital symmetries:

Alpha Orbitals:

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The electronic state of the initial guess is 2-A'.

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

Leave Link 401 at Sun Aug 18 13:41:15 2019, MaxMem= 2013265920 cpu: 21.4

(Enter /home/kira/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3047318 IEndB= 3047318 NGot= 2013265920 MDV= 2011240249

LenX= 2011240249 LenY= 2010235243

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= 480000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 98911692.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.66D-15 for 5738.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.57D-15 for 4797 2561.

Iteration 1 A^-1\*A deviation from unit magnitude is 8.66D-15 for 5738.

Iteration 1 A^-1\*A deviation from orthogonality is 6.14D-13 for 4232 4220.

E= -1913.46235926724

DIIS: error= 4.65D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1913.46235926724 IErMin= 1 ErrMin= 4.65D-02

ErrMax= 4.65D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.28D+00 BMatP= 4.28D+00

IDIUse=3 WtCom= 5.35D-01 WtEn= 4.65D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.031 Goal= None Shift= 0.000

Gap= 0.103 Goal= None Shift= 0.000

GapD= 0.031 DampG=0.250 DampE=0.500 DampFc=0.2500 IDamp=-1.

Damping current iteration by 2.50D-01

RMSDP=2.10D-03 MaxDP=1.09D-01 OVMax= 2.30D-01

Cycle 2 Pass 1 IDiag 1:

RMSU= 5.21D-04 CP: 9.90D-01

E= -1913.82299022664 Delta-E= -0.360630959398 Rises=F Damp=T

DIIS: error= 2.61D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1913.82299022664 IErMin= 2 ErrMin= 2.61D-02

ErrMax= 2.61D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.37D+00 BMatP= 4.28D+00

IDIUse=3 WtCom= 7.39D-01 WtEn= 2.61D-01

Coeff-Com: -0.113D+01 0.213D+01

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

Coeff: -0.833D+00 0.183D+01

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=7.30D-04 MaxDP=3.50D-02 DE=-3.61D-01 OVMax= 1.38D-01

Cycle 3 Pass 1 IDiag 1:

RMSU= 4.59D-04 CP: 9.76D-01 2.08D+00

E= -1914.46849846435 Delta-E= -0.645508237718 Rises=F Damp=F

DIIS: error= 4.13D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.46849846435 IErMin= 3 ErrMin= 4.13D-03

ErrMax= 4.13D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.53D-02 BMatP= 1.37D+00

IDIUse=3 WtCom= 9.59D-01 WtEn= 4.13D-02

Coeff-Com: -0.332D+00 0.669D+00 0.663D+00

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

Coeff: -0.318D+00 0.642D+00 0.677D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=2.65D-04 MaxDP=1.48D-02 DE=-6.46D-01 OVMax= 5.11D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.06D-04 CP: 9.80D-01 2.02D+00 6.46D-01

E= -1914.48252239561 Delta-E= -0.014023931254 Rises=F Damp=F

DIIS: error= 3.22D-03 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.48252239561 IErMin= 4 ErrMin= 3.22D-03

ErrMax= 3.22D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.17D-02 BMatP= 8.53D-02

IDIUse=3 WtCom= 9.68D-01 WtEn= 3.22D-02

Coeff-Com: -0.375D-01 0.933D-01 0.388D+00 0.556D+00

Coeff-En: 0.000D+00 0.000D+00 0.274D+00 0.726D+00

Coeff: -0.363D-01 0.903D-01 0.384D+00 0.562D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=1.34D-04 MaxDP=6.61D-03 DE=-1.40D-02 OVMax= 2.38D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 7.13D-05 CP: 9.78D-01 1.98D+00 7.50D-01 5.20D-01

E= -1914.49019827660 Delta-E= -0.007675880997 Rises=F Damp=F

DIIS: error= 1.04D-03 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.49019827660 IErMin= 5 ErrMin= 1.04D-03

ErrMax= 1.04D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.44D-03 BMatP= 3.17D-02

IDIUse=3 WtCom= 9.90D-01 WtEn= 1.04D-02

Coeff-Com: 0.228D-02 0.336D-02 0.160D+00 0.307D+00 0.527D+00

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

Coeff: 0.225D-02 0.333D-02 0.158D+00 0.304D+00 0.532D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=4.32D-05 MaxDP=2.71D-03 DE=-7.68D-03 OVMax= 9.87D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.03D-05 CP: 9.78D-01 2.00D+00 7.63D-01 5.89D-01 5.54D-01

E= -1914.49071522196 Delta-E= -0.000516945353 Rises=F Damp=F

DIIS: error= 3.23D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.49071522196 IErMin= 6 ErrMin= 3.23D-04

ErrMax= 3.23D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.04D-04 BMatP= 2.44D-03

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.23D-03

Coeff-Com: 0.380D-02-0.514D-02 0.516D-01 0.117D+00 0.312D+00 0.521D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.740D-01 0.926D+00

Coeff: 0.379D-02-0.512D-02 0.514D-01 0.117D+00 0.311D+00 0.522D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=1.14D-05 MaxDP=7.78D-04 DE=-5.17D-04 OVMax= 3.45D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.80D-06 CP: 9.78D-01 2.00D+00 7.62D-01 5.87D-01 6.40D-01

CP: 6.59D-01

E= -1914.49078758538 Delta-E= -0.000072363418 Rises=F Damp=F

DIIS: error= 9.40D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.49078758538 IErMin= 7 ErrMin= 9.40D-05

ErrMax= 9.40D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.73D-05 BMatP= 3.04D-04

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

Coeff-Com: 0.202D-02-0.318D-02 0.167D-01 0.413D-01 0.128D+00 0.270D+00

Coeff-Com: 0.545D+00

Coeff: 0.202D-02-0.318D-02 0.167D-01 0.413D-01 0.128D+00 0.270D+00

Coeff: 0.545D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=2.99D-06 MaxDP=1.81D-04 DE=-7.24D-05 OVMax= 8.31D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.35D-06 CP: 9.78D-01 2.00D+00 7.63D-01 5.90D-01 6.41D-01

CP: 6.96D-01 7.39D-01

E= -1914.49079198127 Delta-E= -0.000004395897 Rises=F Damp=F

DIIS: error= 3.61D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.49079198127 IErMin= 8 ErrMin= 3.61D-05

ErrMax= 3.61D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.93D-06 BMatP= 1.73D-05

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

Coeff-Com: 0.109D-03-0.306D-03-0.488D-02-0.101D-01-0.200D-01-0.785D-02

Coeff-Com: 0.218D+00 0.825D+00

Coeff: 0.109D-03-0.306D-03-0.488D-02-0.101D-01-0.200D-01-0.785D-02

Coeff: 0.218D+00 0.825D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=1.34D-06 MaxDP=1.11D-04 DE=-4.40D-06 OVMax= 5.41D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 8.52D-07 CP: 9.78D-01 2.00D+00 7.63D-01 5.90D-01 6.47D-01

CP: 7.10D-01 8.84D-01 1.07D+00

E= -1914.49079286899 Delta-E= -0.000000887713 Rises=F Damp=F

DIIS: error= 1.55D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.49079286899 IErMin= 9 ErrMin= 1.55D-05

ErrMax= 1.55D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.26D-07 BMatP= 1.93D-06

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

Coeff-Com: -0.236D-03 0.314D-03-0.424D-02-0.100D-01-0.256D-01-0.377D-01

Coeff-Com: 0.220D-01 0.361D+00 0.694D+00

Coeff: -0.236D-03 0.314D-03-0.424D-02-0.100D-01-0.256D-01-0.377D-01

Coeff: 0.220D-01 0.361D+00 0.694D+00

Gap= 0.041 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=5.93D-07 MaxDP=5.32D-05 DE=-8.88D-07 OVMax= 2.33D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 4.23D-07 CP: 9.78D-01 2.00D+00 7.63D-01 5.90D-01 6.47D-01

CP: 7.18D-01 9.17D-01 1.20D+00 1.01D+00

E= -1914.49079306785 Delta-E= -0.000000198860 Rises=F Damp=F

DIIS: error= 8.20D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.49079306785 IErMin=10 ErrMin= 8.20D-06

ErrMax= 8.20D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.20D-07 BMatP= 4.26D-07

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

Coeff-Com: -0.164D-03 0.276D-03-0.229D-03-0.122D-02-0.505D-02-0.150D-01

Coeff-Com: -0.745D-01-0.145D+00 0.353D+00 0.888D+00

Coeff: -0.164D-03 0.276D-03-0.229D-03-0.122D-02-0.505D-02-0.150D-01

Coeff: -0.745D-01-0.145D+00 0.353D+00 0.888D+00

Gap= 0.041 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=4.08D-07 MaxDP=4.16D-05 DE=-1.99D-07 OVMax= 1.48D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.94D-07 CP: 9.78D-01 2.00D+00 7.63D-01 5.90D-01 6.48D-01

CP: 7.21D-01 9.41D-01 1.29D+00 1.30D+00 1.04D+00

E= -1914.49079314232 Delta-E= -0.000000074474 Rises=F Damp=F

DIIS: error= 1.85D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.49079314232 IErMin=11 ErrMin= 1.85D-06

ErrMax= 1.85D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.51D-08 BMatP= 1.20D-07

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

Coeff-Com: -0.490D-04 0.873D-04 0.274D-03 0.421D-03 0.238D-03-0.309D-02

Coeff-Com: -0.335D-01-0.964D-01 0.907D-01 0.387D+00 0.654D+00

Coeff: -0.490D-04 0.873D-04 0.274D-03 0.421D-03 0.238D-03-0.309D-02

Coeff: -0.335D-01-0.964D-01 0.907D-01 0.387D+00 0.654D+00

Gap= 0.041 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=1.06D-07 MaxDP=8.21D-06 DE=-7.45D-08 OVMax= 3.39D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 7.75D-08 CP: 9.78D-01 2.00D+00 7.63D-01 5.90D-01 6.48D-01

CP: 7.21D-01 9.39D-01 1.30D+00 1.34D+00 1.16D+00

CP: 1.05D+00

E= -1914.49079314923 Delta-E= -0.000000006909 Rises=F Damp=F

DIIS: error= 1.75D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.49079314923 IErMin=12 ErrMin= 1.75D-06

ErrMax= 1.75D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.53D-09 BMatP= 1.51D-08

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

Coeff-Com: 0.235D-04-0.361D-04 0.217D-03 0.628D-03 0.168D-02 0.272D-02

Coeff-Com: 0.485D-02-0.851D-02-0.584D-01-0.631D-01 0.345D+00 0.775D+00

Coeff: 0.235D-04-0.361D-04 0.217D-03 0.628D-03 0.168D-02 0.272D-02

Coeff: 0.485D-02-0.851D-02-0.584D-01-0.631D-01 0.345D+00 0.775D+00

Gap= 0.041 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=7.10D-08 MaxDP=4.90D-06 DE=-6.91D-09 OVMax= 2.41D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 3.65D-08 CP: 9.78D-01 2.00D+00 7.63D-01 5.90D-01 6.48D-01

CP: 7.21D-01 9.40D-01 1.30D+00 1.36D+00 1.21D+00

CP: 1.32D+00 1.05D+00

E= -1914.49079315228 Delta-E= -0.000000003054 Rises=F Damp=F

DIIS: error= 1.41D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1914.49079315228 IErMin=13 ErrMin= 1.41D-06

ErrMax= 1.41D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.65D-10 BMatP= 4.53D-09

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

Coeff-Com: 0.166D-04-0.271D-04 0.401D-04 0.179D-03 0.622D-03 0.163D-02

Coeff-Com: 0.753D-02 0.126D-01-0.400D-01-0.901D-01 0.407D-01 0.339D+00

Coeff-Com: 0.728D+00

Coeff: 0.166D-04-0.271D-04 0.401D-04 0.179D-03 0.622D-03 0.163D-02

Coeff: 0.753D-02 0.126D-01-0.400D-01-0.901D-01 0.407D-01 0.339D+00

Coeff: 0.728D+00

Gap= 0.041 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=3.49D-08 MaxDP=1.49D-06 DE=-3.05D-09 OVMax= 1.14D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 2.11D-08 CP: 9.78D-01 2.00D+00 7.63D-01 5.90D-01 6.48D-01

CP: 7.21D-01 9.40D-01 1.30D+00 1.37D+00 1.24D+00

CP: 1.39D+00 1.29D+00 1.16D+00

E= -1914.49079315309 Delta-E= -0.000000000805 Rises=F Damp=F

DIIS: error= 9.77D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1914.49079315309 IErMin=14 ErrMin= 9.77D-07

ErrMax= 9.77D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.58D-10 BMatP= 9.65D-10

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

Coeff-Com: 0.139D-05-0.297D-05-0.713D-04-0.181D-03-0.402D-03-0.232D-03

Coeff-Com: 0.207D-02 0.119D-01 0.431D-02-0.245D-01-0.155D+00-0.184D+00

Coeff-Com: 0.487D+00 0.860D+00

Coeff: 0.139D-05-0.297D-05-0.713D-04-0.181D-03-0.402D-03-0.232D-03

Coeff: 0.207D-02 0.119D-01 0.431D-02-0.245D-01-0.155D+00-0.184D+00

Coeff: 0.487D+00 0.860D+00

Gap= 0.041 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=3.02D-08 MaxDP=1.17D-06 DE=-8.05D-10 OVMax= 1.02D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 1.14D-08 CP: 9.78D-01 2.00D+00 7.63D-01 5.90D-01 6.48D-01

CP: 7.21D-01 9.40D-01 1.30D+00 1.37D+00 1.25D+00

CP: 1.47D+00 1.42D+00 1.64D+00 1.16D+00

E= -1914.49079315351 Delta-E= -0.000000000419 Rises=F Damp=F

DIIS: error= 2.71D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1914.49079315351 IErMin=15 ErrMin= 2.71D-07

ErrMax= 2.71D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.42D-11 BMatP= 4.58D-10

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

Coeff-Com: -0.409D-05 0.631D-05-0.188D-04-0.663D-04-0.189D-03-0.402D-03

Coeff-Com: -0.140D-02-0.139D-02 0.866D-02 0.165D-01-0.226D-01-0.866D-01

Coeff-Com: -0.103D+00 0.933D-01 0.110D+01

Coeff: -0.409D-05 0.631D-05-0.188D-04-0.663D-04-0.189D-03-0.402D-03

Coeff: -0.140D-02-0.139D-02 0.866D-02 0.165D-01-0.226D-01-0.866D-01

Coeff: -0.103D+00 0.933D-01 0.110D+01

Gap= 0.041 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=1.30D-08 MaxDP=5.15D-07 DE=-4.19D-10 OVMax= 4.33D-06

Cycle 16 Pass 1 IDiag 1:

RMSU= 5.33D-09 CP: 9.78D-01 2.00D+00 7.63D-01 5.90D-01 6.48D-01

CP: 7.21D-01 9.40D-01 1.30D+00 1.38D+00 1.26D+00

CP: 1.49D+00 1.48D+00 1.84D+00 1.44D+00 1.42D+00

E= -1914.49079315356 Delta-E= -0.000000000049 Rises=F Damp=F

DIIS: error= 9.16D-08 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1914.49079315356 IErMin=16 ErrMin= 9.16D-08

ErrMax= 9.16D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.72D-11 BMatP= 4.42D-11

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

Coeff-Com: -0.237D-05 0.384D-05 0.456D-05 0.427D-05-0.851D-05-0.143D-03

Coeff-Com: -0.100D-02-0.289D-02 0.289D-02 0.117D-01 0.213D-01-0.152D-02

Coeff-Com: -0.149D+00-0.132D+00 0.518D+00 0.732D+00

Coeff: -0.237D-05 0.384D-05 0.456D-05 0.427D-05-0.851D-05-0.143D-03

Coeff: -0.100D-02-0.289D-02 0.289D-02 0.117D-01 0.213D-01-0.152D-02

Coeff: -0.149D+00-0.132D+00 0.518D+00 0.732D+00

Gap= 0.041 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=5.20D-09 MaxDP=2.12D-07 DE=-4.91D-11 OVMax= 1.62D-06

Error on total polarization charges = 0.08602

SCF Done: E(UB3LYP) = -1914.49079315 A.U. after 16 cycles

NFock= 16 Conv=0.52D-08 -V/T= 2.0041

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7586 S= 0.5043

<L.S>= 0.000000000000E+00

KE= 1.906691750895D+03 PE=-1.520414306317D+04 EE= 6.023356300197D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.33

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7586, after 0.7501

Leave Link 502 at Sun Aug 18 13:50:50 2019, MaxMem= 2013265920 cpu: 4584.8

(Enter /home/kira/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:

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The electronic state is 2-A'.

Alpha occ. eigenvalues -- -14.33462 -14.33418 -14.26849 -14.26849 -10.20709

Alpha occ. eigenvalues -- -10.20709 -10.20698 -10.20698 -10.18002 -10.18002

Alpha occ. eigenvalues -- -10.17999 -10.17998 -10.17983 -10.17983 -10.17980

Alpha occ. eigenvalues -- -10.17980 -10.17666 -10.17666 -10.17662 -10.17662

Alpha occ. eigenvalues -- -10.16886 -10.16886 -10.16886 -10.16885 -10.16857

Alpha occ. eigenvalues -- -10.16857 -10.16857 -10.16857 -10.16811 -10.16811

Alpha occ. eigenvalues -- -10.16811 -10.16811 -10.16787 -10.16787 -10.16786

Alpha occ. eigenvalues -- -10.16786 -10.16756 -10.16756 -10.16756 -10.16756

Alpha occ. eigenvalues -- -10.16644 -10.16641 -10.16579 -10.16576 -10.14315

Alpha occ. eigenvalues -- -10.14315 -10.14256 -10.14256 -0.97703 -0.97569

Alpha occ. eigenvalues -- -0.92702 -0.92443 -0.86325 -0.86048 -0.86005

Alpha occ. eigenvalues -- -0.85884 -0.81453 -0.80112 -0.79606 -0.78963

Alpha occ. eigenvalues -- -0.78227 -0.77321 -0.74823 -0.74593 -0.74568

Alpha occ. eigenvalues -- -0.74508 -0.74268 -0.73769 -0.73627 -0.72746

Alpha occ. eigenvalues -- -0.72384 -0.70725 -0.70055 -0.65320 -0.65313

Alpha occ. eigenvalues -- -0.61637 -0.60658 -0.60463 -0.60315 -0.60183

Alpha occ. eigenvalues -- -0.59513 -0.59376 -0.59314 -0.58755 -0.58739

Alpha occ. eigenvalues -- -0.58414 -0.56167 -0.55863 -0.55131 -0.54026

Alpha occ. eigenvalues -- -0.53421 -0.51687 -0.51566 -0.51471 -0.49724

Alpha occ. eigenvalues -- -0.49541 -0.49366 -0.48842 -0.47849 -0.45975

Alpha occ. eigenvalues -- -0.45620 -0.45293 -0.45227 -0.45224 -0.44617

Alpha occ. eigenvalues -- -0.44558 -0.44426 -0.43911 -0.43399 -0.42894

Alpha occ. eigenvalues -- -0.42406 -0.42132 -0.41936 -0.41931 -0.41866

Alpha occ. eigenvalues -- -0.41703 -0.41615 -0.41372 -0.41285 -0.40988

Alpha occ. eigenvalues -- -0.40466 -0.39625 -0.38881 -0.38479 -0.38241

Alpha occ. eigenvalues -- -0.38007 -0.37527 -0.37088 -0.37003 -0.36592

Alpha occ. eigenvalues -- -0.36152 -0.35988 -0.35495 -0.35252 -0.34722

Alpha occ. eigenvalues -- -0.34224 -0.34180 -0.34166 -0.34141 -0.34136

Alpha occ. eigenvalues -- -0.33770 -0.33301 -0.31161 -0.28663 -0.27690

Alpha occ. eigenvalues -- -0.26631 -0.26309 -0.26237 -0.25933 -0.25657

Alpha occ. eigenvalues -- -0.25600 -0.25508 -0.25402 -0.25390 -0.24721

Alpha occ. eigenvalues -- -0.24586 -0.24216 -0.22784 -0.22515 -0.19926

Alpha occ. eigenvalues -- -0.18211 -0.11946

Alpha virt. eigenvalues -- -0.07894 -0.03917 -0.00928 -0.00889 -0.00844

Alpha virt. eigenvalues -- -0.00733 -0.00587 -0.00563 -0.00387 -0.00315

Alpha virt. eigenvalues -- 0.03952 0.05606 0.05883 0.05905 0.06000

Alpha virt. eigenvalues -- 0.06180 0.06587 0.07980 0.08039 0.08478

Alpha virt. eigenvalues -- 0.08542 0.08703 0.09497 0.09787 0.09794

Alpha virt. eigenvalues -- 0.10283 0.10331 0.10713 0.10775 0.10833

Alpha virt. eigenvalues -- 0.11132 0.11584 0.12003 0.12460 0.12663

Alpha virt. eigenvalues -- 0.13015 0.13215 0.13259 0.13311 0.13467

Alpha virt. eigenvalues -- 0.13519 0.13605 0.13916 0.14415 0.14549

Alpha virt. eigenvalues -- 0.14608 0.14734 0.16091 0.16477 0.17011

Alpha virt. eigenvalues -- 0.17350 0.18041 0.18701 0.20667 0.22100

Alpha virt. eigenvalues -- 0.22519 0.23675 0.23974 0.24600 0.24776

Alpha virt. eigenvalues -- 0.24991 0.24998 0.25385 0.26109 0.26492

Alpha virt. eigenvalues -- 0.26887 0.27286 0.27350 0.27928 0.28244

Alpha virt. eigenvalues -- 0.28330 0.28357 0.28685 0.28696 0.28855

Alpha virt. eigenvalues -- 0.29392 0.29454 0.30063 0.30069 0.30281

Alpha virt. eigenvalues -- 0.30448 0.30472 0.31416 0.31678 0.31876

Alpha virt. eigenvalues -- 0.31949 0.32578 0.32649 0.34068 0.34774

Alpha virt. eigenvalues -- 0.35117 0.35751 0.36199 0.36337 0.36446

Alpha virt. eigenvalues -- 0.36755 0.37020 0.37085 0.37485 0.37738

Alpha virt. eigenvalues -- 0.38032 0.38156 0.38302 0.38630 0.38660

Alpha virt. eigenvalues -- 0.39170 0.39204 0.39430 0.39613 0.40205

Alpha virt. eigenvalues -- 0.40664 0.40715 0.40909 0.41049 0.41159

Alpha virt. eigenvalues -- 0.41324 0.41454 0.41724 0.41853 0.41991

Alpha virt. eigenvalues -- 0.42134 0.42356 0.42469 0.42536 0.42546

Alpha virt. eigenvalues -- 0.43240 0.43383 0.43395 0.43426 0.43937

Alpha virt. eigenvalues -- 0.44069 0.44313 0.44406 0.44838 0.45312

Alpha virt. eigenvalues -- 0.45387 0.45447 0.45483 0.45553 0.45936

Alpha virt. eigenvalues -- 0.46225 0.46331 0.46465 0.46674 0.47130

Alpha virt. eigenvalues -- 0.47608 0.47914 0.47938 0.48084 0.48333

Alpha virt. eigenvalues -- 0.48590 0.48726 0.49229 0.49627 0.50203

Alpha virt. eigenvalues -- 0.50375 0.50416 0.51148 0.51636 0.51693

Alpha virt. eigenvalues -- 0.52597 0.52758 0.53362 0.53383 0.53766

Alpha virt. eigenvalues -- 0.53895 0.54379 0.54658 0.54723 0.55463

Alpha virt. eigenvalues -- 0.55881 0.55942 0.56942 0.58269 0.58270

Alpha virt. eigenvalues -- 0.58648 0.58667 0.58858 0.58913 0.59443

Alpha virt. eigenvalues -- 0.59967 0.60264 0.60311 0.60716 0.60749

Alpha virt. eigenvalues -- 0.60788 0.60891 0.61156 0.61344 0.61352

Alpha virt. eigenvalues -- 0.61606 0.61778 0.61879 0.61945 0.62109

Alpha virt. eigenvalues -- 0.62495 0.62621 0.63059 0.63086 0.63296

Alpha virt. eigenvalues -- 0.63451 0.64237 0.64514 0.64667 0.65115

Alpha virt. eigenvalues -- 0.65303 0.65479 0.65745 0.65805 0.66002

Alpha virt. eigenvalues -- 0.66038 0.66076 0.66406 0.66692 0.67119

Alpha virt. eigenvalues -- 0.68166 0.68687 0.69298 0.69638 0.69934

Alpha virt. eigenvalues -- 0.70187 0.70886 0.71232 0.71574 0.71881

Alpha virt. eigenvalues -- 0.72784 0.72885 0.73209 0.73229 0.73796

Alpha virt. eigenvalues -- 0.73822 0.74374 0.74456 0.74654 0.74803

Alpha virt. eigenvalues -- 0.74940 0.75717 0.75858 0.76012 0.76524

Alpha virt. eigenvalues -- 0.76689 0.76757 0.77224 0.77710 0.78321

Alpha virt. eigenvalues -- 0.79159 0.79235 0.79268 0.79370 0.79644

Alpha virt. eigenvalues -- 0.79810 0.80141 0.80552 0.81001 0.81173

Alpha virt. eigenvalues -- 0.81488 0.82365 0.82437 0.82677 0.82736

Alpha virt. eigenvalues -- 0.84405 0.84486 0.84645 0.85380 0.85672

Alpha virt. eigenvalues -- 0.86259 0.86322 0.87791 0.88056 0.88091

Alpha virt. eigenvalues -- 0.88712 0.89147 0.89292 0.89678 0.89814

Alpha virt. eigenvalues -- 0.89840 0.91827 0.91844 0.92704 0.93007

Alpha virt. eigenvalues -- 0.93086 0.93823 0.94347 0.94528 0.94821

Alpha virt. eigenvalues -- 0.95994 0.96314 0.96422 0.96932 0.97060

Alpha virt. eigenvalues -- 0.98302 0.98951 0.99668 1.00261 1.00822

Alpha virt. eigenvalues -- 1.01447 1.01810 1.02183 1.02552 1.03022

Alpha virt. eigenvalues -- 1.03428 1.03485 1.03714 1.04207 1.05342

Alpha virt. eigenvalues -- 1.05786 1.06971 1.08083 1.08909 1.09717

Alpha virt. eigenvalues -- 1.09837 1.10028 1.10411 1.11477 1.12466

Alpha virt. eigenvalues -- 1.13191 1.14266 1.14649 1.14784 1.14880

Alpha virt. eigenvalues -- 1.15000 1.15083 1.16090 1.16637 1.16841

Alpha virt. eigenvalues -- 1.17110 1.17482 1.17690 1.17968 1.19623

Alpha virt. eigenvalues -- 1.19674 1.19704 1.20158 1.20925 1.21244

Alpha virt. eigenvalues -- 1.21358 1.21486 1.22100 1.22103 1.22583

Alpha virt. eigenvalues -- 1.22856 1.23791 1.23846 1.24005 1.24981

Alpha virt. eigenvalues -- 1.25720 1.25894 1.26255 1.26843 1.26859

Alpha virt. eigenvalues -- 1.27399 1.27883 1.28203 1.28331 1.29434

Alpha virt. eigenvalues -- 1.30677 1.30813 1.31289 1.32185 1.32993

Alpha virt. eigenvalues -- 1.33197 1.33306 1.34346 1.35171 1.36585

Alpha virt. eigenvalues -- 1.38175 1.39216 1.40727 1.41150 1.41403

Alpha virt. eigenvalues -- 1.42422 1.42491 1.42683 1.42727 1.44864

Alpha virt. eigenvalues -- 1.45937 1.46159 1.46512 1.47713 1.47919

Alpha virt. eigenvalues -- 1.48197 1.48547 1.48609 1.48891 1.48978

Alpha virt. eigenvalues -- 1.49149 1.49538 1.50092 1.50119 1.50520

Alpha virt. eigenvalues -- 1.52465 1.53515 1.53734 1.53992 1.54006

Alpha virt. eigenvalues -- 1.54509 1.54900 1.55314 1.55951 1.58639

Alpha virt. eigenvalues -- 1.58709 1.60041 1.62524 1.62643 1.62978

Alpha virt. eigenvalues -- 1.63433 1.64353 1.65068 1.65627 1.66051

Alpha virt. eigenvalues -- 1.68654 1.68685 1.68689 1.69181 1.69213

Alpha virt. eigenvalues -- 1.70091 1.70619 1.71221 1.71325 1.72106

Alpha virt. eigenvalues -- 1.72562 1.74895 1.74925 1.74995 1.75608

Alpha virt. eigenvalues -- 1.75694 1.75826 1.76383 1.76823 1.76933

Alpha virt. eigenvalues -- 1.77988 1.78536 1.79541 1.79834 1.80224

Alpha virt. eigenvalues -- 1.80485 1.80949 1.81262 1.81540 1.82118

Alpha virt. eigenvalues -- 1.82581 1.82687 1.82742 1.83593 1.83627

Alpha virt. eigenvalues -- 1.84475 1.84991 1.85159 1.86295 1.86337

Alpha virt. eigenvalues -- 1.86411 1.88280 1.88596 1.89011 1.89026

Alpha virt. eigenvalues -- 1.89702 1.89858 1.90904 1.91087 1.91952

Alpha virt. eigenvalues -- 1.92246 1.92469 1.92609 1.92770 1.92922

Alpha virt. eigenvalues -- 1.93039 1.93412 1.93741 1.94014 1.94197

Alpha virt. eigenvalues -- 1.94516 1.94581 1.94912 1.95465 1.95477

Alpha virt. eigenvalues -- 1.95606 1.96857 1.97140 1.97369 1.97455

Alpha virt. eigenvalues -- 1.97595 1.98298 1.98470 1.98868 2.00355

Alpha virt. eigenvalues -- 2.00689 2.01472 2.02107 2.02728 2.03066

Alpha virt. eigenvalues -- 2.07297 2.07876 2.08106 2.09733 2.09980

Alpha virt. eigenvalues -- 2.10285 2.11309 2.11590 2.14282 2.14874

Alpha virt. eigenvalues -- 2.15044 2.18396 2.19303 2.22965 2.24131

Alpha virt. eigenvalues -- 2.24759 2.24903 2.25280 2.25743 2.26293

Alpha virt. eigenvalues -- 2.26440 2.27060 2.27230 2.27316 2.27632

Alpha virt. eigenvalues -- 2.27920 2.27932 2.28217 2.28364 2.28417

Alpha virt. eigenvalues -- 2.28583 2.29268 2.29980 2.30014 2.30454

Alpha virt. eigenvalues -- 2.30906 2.31182 2.31918 2.32595 2.33257

Alpha virt. eigenvalues -- 2.33556 2.33759 2.33868 2.35631 2.35790

Alpha virt. eigenvalues -- 2.35951 2.36525 2.37554 2.37578 2.37669

Alpha virt. eigenvalues -- 2.38221 2.39796 2.40131 2.40470 2.40998

Alpha virt. eigenvalues -- 2.41108 2.42140 2.44394 2.44718 2.45856

Alpha virt. eigenvalues -- 2.46076 2.48525 2.48901 2.49575 2.52436

Alpha virt. eigenvalues -- 2.52710 2.53766 2.54152 2.54231 2.55244

Alpha virt. eigenvalues -- 2.57303 2.57671 2.58320 2.58823 2.59079

Alpha virt. eigenvalues -- 2.59494 2.59793 2.60846 2.61234 2.62769

Alpha virt. eigenvalues -- 2.63206 2.63260 2.63978 2.65317 2.65401

Alpha virt. eigenvalues -- 2.66268 2.66305 2.66609 2.68610 2.68713

Alpha virt. eigenvalues -- 2.70523 2.70841 2.70924 2.71281 2.72139

Alpha virt. eigenvalues -- 2.73457 2.73625 2.74169 2.74879 2.75055

Alpha virt. eigenvalues -- 2.75944 2.76024 2.77877 2.77954 2.78275

Alpha virt. eigenvalues -- 2.78772 2.79377 2.79600 2.79931 2.80671

Alpha virt. eigenvalues -- 2.83456 2.84209 2.84311 2.84321 2.85179

Alpha virt. eigenvalues -- 2.86426 2.86723 2.87132 2.87927 2.90368

Alpha virt. eigenvalues -- 2.91002 2.91105 2.91561 2.93000 2.95783

Alpha virt. eigenvalues -- 2.96332 2.96600 2.98717 2.99611 2.99765

Alpha virt. eigenvalues -- 3.00198 3.01209 3.03628 3.04391 3.04434

Alpha virt. eigenvalues -- 3.05136 3.05676 3.06496 3.06701 3.08253

Alpha virt. eigenvalues -- 3.08727 3.09288 3.09722 3.09805 3.11357

Alpha virt. eigenvalues -- 3.11717 3.13171 3.13192 3.15012 3.16374

Alpha virt. eigenvalues -- 3.16616 3.17752 3.18125 3.19053 3.20608

Alpha virt. eigenvalues -- 3.21174 3.23304 3.25032 3.25062 3.25863

Alpha virt. eigenvalues -- 3.26493 3.26730 3.26990 3.28362 3.28847

Alpha virt. eigenvalues -- 3.30174 3.30344 3.30551 3.30794 3.31141

Alpha virt. eigenvalues -- 3.31245 3.31314 3.31315 3.31856 3.32186

Alpha virt. eigenvalues -- 3.32601 3.32905 3.33111 3.34061 3.34268

Alpha virt. eigenvalues -- 3.34486 3.35964 3.36460 3.37328 3.37888

Alpha virt. eigenvalues -- 3.37948 3.38733 3.40144 3.41127 3.42769

Alpha virt. eigenvalues -- 3.43933 3.44109 3.46442 3.46511 3.49703

Alpha virt. eigenvalues -- 3.51601 3.51868 3.52623 3.57708 3.57735

Alpha virt. eigenvalues -- 3.58986 3.59080 3.59190 3.60863 3.62372

Alpha virt. eigenvalues -- 3.63188 3.64383 3.66118 3.66200 3.67464

Alpha virt. eigenvalues -- 3.72576 3.72810 3.73130 3.75644 3.77442

Alpha virt. eigenvalues -- 3.78821 3.82321 3.82808 3.84622 3.85578

Alpha virt. eigenvalues -- 3.90131 3.91865 3.92975 3.94232 3.94470

Alpha virt. eigenvalues -- 3.94946 3.96545 3.96719 3.97001 3.97256

Alpha virt. eigenvalues -- 3.99691 4.00222 4.04520 4.12051 4.30823

Alpha virt. eigenvalues -- 4.31946 4.38192 4.42037 4.49164 4.53302

Alpha virt. eigenvalues -- 4.56273 4.57358 4.65006 4.65239 4.68537

Alpha virt. eigenvalues -- 4.70077 4.79224 4.79238 4.79247 4.79263

Alpha virt. eigenvalues -- 5.10883 5.17036 5.18624 5.28685 23.25447

Alpha virt. eigenvalues -- 23.28948 23.29056 23.30755 23.47390 23.53813

Alpha virt. eigenvalues -- 23.55546 23.60904 23.76387 23.79001 23.79384

Alpha virt. eigenvalues -- 23.81144 23.81343 23.81345 23.81613 23.82296

Alpha virt. eigenvalues -- 23.86260 23.86968 23.87004 23.87617 23.92237

Alpha virt. eigenvalues -- 23.93273 23.96487 23.97644 23.99869 23.99995

Alpha virt. eigenvalues -- 24.01350 24.01643 24.05565 24.05698 24.05746

Alpha virt. eigenvalues -- 24.05898 24.08311 24.08565 24.10049 24.10149

Alpha virt. eigenvalues -- 24.13688 24.13991 24.14017 24.14602 24.16215

Alpha virt. eigenvalues -- 24.16282 24.16283 24.16383 35.57848 35.58743

Alpha virt. eigenvalues -- 35.65286 35.65818

Beta occ. eigenvalues -- -14.33316 -14.33271 -14.26902 -14.26902 -10.20694

Beta occ. eigenvalues -- -10.20694 -10.20683 -10.20683 -10.18015 -10.18014

Beta occ. eigenvalues -- -10.18011 -10.18010 -10.17864 -10.17864 -10.17862

Beta occ. eigenvalues -- -10.17862 -10.17550 -10.17550 -10.17546 -10.17546

Beta occ. eigenvalues -- -10.16885 -10.16885 -10.16885 -10.16884 -10.16858

Beta occ. eigenvalues -- -10.16858 -10.16857 -10.16857 -10.16802 -10.16801

Beta occ. eigenvalues -- -10.16801 -10.16801 -10.16774 -10.16774 -10.16774

Beta occ. eigenvalues -- -10.16774 -10.16746 -10.16746 -10.16745 -10.16745

Beta occ. eigenvalues -- -10.16640 -10.16637 -10.16576 -10.16572 -10.14222

Beta occ. eigenvalues -- -10.14222 -10.14162 -10.14162 -0.97522 -0.97388

Beta occ. eigenvalues -- -0.92536 -0.92279 -0.86261 -0.86005 -0.85965

Beta occ. eigenvalues -- -0.85852 -0.81255 -0.79929 -0.79405 -0.78828

Beta occ. eigenvalues -- -0.78124 -0.77225 -0.74748 -0.74571 -0.74536

Beta occ. eigenvalues -- -0.74488 -0.74188 -0.73582 -0.73580 -0.72644

Beta occ. eigenvalues -- -0.72245 -0.70485 -0.69889 -0.65252 -0.64948

Beta occ. eigenvalues -- -0.61543 -0.60622 -0.60444 -0.60287 -0.60157

Beta occ. eigenvalues -- -0.59435 -0.59306 -0.59288 -0.58701 -0.58614

Beta occ. eigenvalues -- -0.58312 -0.56134 -0.55725 -0.55040 -0.53890

Beta occ. eigenvalues -- -0.53294 -0.51606 -0.51545 -0.51382 -0.49624

Beta occ. eigenvalues -- -0.49479 -0.49270 -0.48744 -0.47789 -0.45942

Beta occ. eigenvalues -- -0.45566 -0.45184 -0.45180 -0.45154 -0.44563

Beta occ. eigenvalues -- -0.44525 -0.44352 -0.43880 -0.43368 -0.42804

Beta occ. eigenvalues -- -0.42209 -0.42031 -0.41910 -0.41882 -0.41857

Beta occ. eigenvalues -- -0.41584 -0.41461 -0.41336 -0.41069 -0.40886

Beta occ. eigenvalues -- -0.40410 -0.39537 -0.38449 -0.38360 -0.38190

Beta occ. eigenvalues -- -0.37491 -0.37446 -0.36971 -0.36949 -0.36532

Beta occ. eigenvalues -- -0.36059 -0.35921 -0.35372 -0.35127 -0.34690

Beta occ. eigenvalues -- -0.34194 -0.34151 -0.34144 -0.34105 -0.34086

Beta occ. eigenvalues -- -0.33725 -0.33251 -0.30525 -0.28057 -0.27168

Beta occ. eigenvalues -- -0.26387 -0.26071 -0.25925 -0.25911 -0.25577

Beta occ. eigenvalues -- -0.25552 -0.25470 -0.25283 -0.25266 -0.24631

Beta occ. eigenvalues -- -0.24441 -0.23704 -0.22370 -0.22200 -0.18829

Beta occ. eigenvalues -- -0.17176

Beta virt. eigenvalues -- -0.08155 -0.07706 -0.02936 -0.00848 -0.00825

Beta virt. eigenvalues -- -0.00784 -0.00688 -0.00548 -0.00458 -0.00355

Beta virt. eigenvalues -- -0.00060 0.04553 0.05635 0.05893 0.05915

Beta virt. eigenvalues -- 0.06188 0.06813 0.06837 0.08061 0.08447

Beta virt. eigenvalues -- 0.08494 0.08557 0.08721 0.09506 0.09804

Beta virt. eigenvalues -- 0.09806 0.10297 0.10357 0.10732 0.10796

Beta virt. eigenvalues -- 0.10865 0.11597 0.11693 0.12444 0.12715

Beta virt. eigenvalues -- 0.12783 0.13065 0.13273 0.13325 0.13513

Beta virt. eigenvalues -- 0.13535 0.13579 0.13626 0.13924 0.14426

Beta virt. eigenvalues -- 0.14568 0.14624 0.14757 0.16401 0.16784

Beta virt. eigenvalues -- 0.17275 0.17586 0.18166 0.18850 0.20724

Beta virt. eigenvalues -- 0.22153 0.22607 0.23791 0.24054 0.24661

Beta virt. eigenvalues -- 0.24880 0.25057 0.25130 0.25478 0.26153

Beta virt. eigenvalues -- 0.26554 0.26991 0.27394 0.27450 0.27986

Beta virt. eigenvalues -- 0.28252 0.28337 0.28369 0.28722 0.28750

Beta virt. eigenvalues -- 0.28906 0.29429 0.29488 0.30083 0.30104

Beta virt. eigenvalues -- 0.30330 0.30503 0.30531 0.31453 0.31761

Beta virt. eigenvalues -- 0.31950 0.31989 0.32701 0.32768 0.34178

Beta virt. eigenvalues -- 0.34869 0.35212 0.35858 0.36254 0.36479

Beta virt. eigenvalues -- 0.36523 0.36877 0.37125 0.37232 0.37620

Beta virt. eigenvalues -- 0.37829 0.38233 0.38266 0.38424 0.38706

Beta virt. eigenvalues -- 0.38740 0.39246 0.39289 0.39538 0.39742

Beta virt. eigenvalues -- 0.40301 0.40748 0.40760 0.41031 0.41114

Beta virt. eigenvalues -- 0.41182 0.41374 0.41620 0.41793 0.41924

Beta virt. eigenvalues -- 0.42047 0.42236 0.42447 0.42568 0.42585

Beta virt. eigenvalues -- 0.42655 0.43300 0.43435 0.43494 0.43528

Beta virt. eigenvalues -- 0.44024 0.44121 0.44382 0.44486 0.44920

Beta virt. eigenvalues -- 0.45371 0.45420 0.45488 0.45577 0.45619

Beta virt. eigenvalues -- 0.46032 0.46303 0.46424 0.46542 0.46778

Beta virt. eigenvalues -- 0.47245 0.47748 0.47986 0.48021 0.48257

Beta virt. eigenvalues -- 0.48480 0.48659 0.48831 0.49327 0.49751

Beta virt. eigenvalues -- 0.50278 0.50474 0.50510 0.51213 0.51672

Beta virt. eigenvalues -- 0.51788 0.52780 0.52928 0.53475 0.53491

Beta virt. eigenvalues -- 0.53855 0.54000 0.54468 0.54740 0.54800

Beta virt. eigenvalues -- 0.55585 0.55988 0.56008 0.57029 0.58352

Beta virt. eigenvalues -- 0.58361 0.58738 0.58774 0.58957 0.59035

Beta virt. eigenvalues -- 0.59489 0.60034 0.60346 0.60385 0.60762

Beta virt. eigenvalues -- 0.60794 0.60821 0.60933 0.61172 0.61364

Beta virt. eigenvalues -- 0.61373 0.61638 0.61823 0.61971 0.62008

Beta virt. eigenvalues -- 0.62137 0.62552 0.62708 0.63133 0.63178

Beta virt. eigenvalues -- 0.63361 0.63550 0.64320 0.64600 0.64742

Beta virt. eigenvalues -- 0.65165 0.65341 0.65531 0.65781 0.65856

Beta virt. eigenvalues -- 0.66038 0.66072 0.66126 0.66448 0.66720

Beta virt. eigenvalues -- 0.67220 0.68251 0.68793 0.69346 0.69794

Beta virt. eigenvalues -- 0.69969 0.70311 0.70916 0.71396 0.71663

Beta virt. eigenvalues -- 0.71947 0.72860 0.73005 0.73278 0.73349

Beta virt. eigenvalues -- 0.73845 0.73905 0.74410 0.74495 0.74687

Beta virt. eigenvalues -- 0.74871 0.75068 0.75739 0.75934 0.76109

Beta virt. eigenvalues -- 0.76596 0.76758 0.76775 0.77255 0.77774

Beta virt. eigenvalues -- 0.78533 0.79226 0.79264 0.79341 0.79409

Beta virt. eigenvalues -- 0.79690 0.79838 0.80183 0.80587 0.81064

Beta virt. eigenvalues -- 0.81236 0.81633 0.82436 0.82490 0.82782

Beta virt. eigenvalues -- 0.82813 0.84482 0.84627 0.84698 0.85404

Beta virt. eigenvalues -- 0.85693 0.86353 0.86407 0.87825 0.88131

Beta virt. eigenvalues -- 0.88198 0.88777 0.89205 0.89367 0.89784

Beta virt. eigenvalues -- 0.89884 0.89914 0.91890 0.91985 0.92776

Beta virt. eigenvalues -- 0.93052 0.93187 0.93899 0.94434 0.94627

Beta virt. eigenvalues -- 0.94868 0.96042 0.96352 0.96511 0.96996

Beta virt. eigenvalues -- 0.97107 0.98397 0.99025 0.99886 1.00314

Beta virt. eigenvalues -- 1.00946 1.01480 1.01843 1.02223 1.02662

Beta virt. eigenvalues -- 1.03145 1.03491 1.03532 1.03767 1.04291

Beta virt. eigenvalues -- 1.05411 1.05867 1.07008 1.08211 1.09011

Beta virt. eigenvalues -- 1.09784 1.09920 1.10114 1.10611 1.11598

Beta virt. eigenvalues -- 1.12618 1.13288 1.14407 1.14779 1.14880

Beta virt. eigenvalues -- 1.14950 1.15063 1.15130 1.16252 1.16708

Beta virt. eigenvalues -- 1.16925 1.17233 1.17568 1.17949 1.18257

Beta virt. eigenvalues -- 1.19712 1.19742 1.19778 1.20219 1.20958

Beta virt. eigenvalues -- 1.21282 1.21420 1.21602 1.22214 1.22241

Beta virt. eigenvalues -- 1.22746 1.22909 1.23860 1.23887 1.24050

Beta virt. eigenvalues -- 1.25045 1.25798 1.25942 1.26361 1.26942

Beta virt. eigenvalues -- 1.27069 1.27536 1.27984 1.28398 1.28406

Beta virt. eigenvalues -- 1.29654 1.30790 1.30974 1.31489 1.32372

Beta virt. eigenvalues -- 1.33056 1.33312 1.33492 1.34468 1.35275

Beta virt. eigenvalues -- 1.36666 1.38291 1.39278 1.40848 1.41280

Beta virt. eigenvalues -- 1.41528 1.42461 1.42664 1.42710 1.42781

Beta virt. eigenvalues -- 1.44962 1.46018 1.46256 1.46578 1.47803

Beta virt. eigenvalues -- 1.48050 1.48233 1.48677 1.48789 1.48957

Beta virt. eigenvalues -- 1.49059 1.49220 1.49610 1.50139 1.50201

Beta virt. eigenvalues -- 1.50572 1.52504 1.53567 1.53770 1.54037

Beta virt. eigenvalues -- 1.54056 1.54545 1.54953 1.55552 1.56018

Beta virt. eigenvalues -- 1.58851 1.58959 1.60103 1.62614 1.62803

Beta virt. eigenvalues -- 1.63039 1.63526 1.64560 1.65213 1.65674

Beta virt. eigenvalues -- 1.66104 1.68799 1.68816 1.68859 1.69274

Beta virt. eigenvalues -- 1.69308 1.70229 1.70695 1.71349 1.71435

Beta virt. eigenvalues -- 1.72189 1.72610 1.75025 1.75036 1.75102

Beta virt. eigenvalues -- 1.75729 1.75793 1.75997 1.76483 1.76880

Beta virt. eigenvalues -- 1.77010 1.78060 1.78685 1.79582 1.80012

Beta virt. eigenvalues -- 1.80402 1.80537 1.80993 1.81380 1.81618

Beta virt. eigenvalues -- 1.82327 1.82682 1.82780 1.82859 1.83690

Beta virt. eigenvalues -- 1.83693 1.84593 1.85086 1.85256 1.86386

Beta virt. eigenvalues -- 1.86414 1.86512 1.88462 1.88703 1.89143

Beta virt. eigenvalues -- 1.89162 1.89865 1.89988 1.90960 1.91240

Beta virt. eigenvalues -- 1.92036 1.92426 1.92504 1.92663 1.92803

Beta virt. eigenvalues -- 1.92944 1.93086 1.93442 1.93808 1.94079

Beta virt. eigenvalues -- 1.94273 1.94619 1.94749 1.95087 1.95596

Beta virt. eigenvalues -- 1.95603 1.95691 1.96963 1.97258 1.97512

Beta virt. eigenvalues -- 1.97573 1.97737 1.98430 1.98825 1.98956

Beta virt. eigenvalues -- 2.00449 2.00832 2.01733 2.02185 2.02859

Beta virt. eigenvalues -- 2.03201 2.07577 2.08012 2.08341 2.09832

Beta virt. eigenvalues -- 2.10226 2.10424 2.11481 2.11631 2.14410

Beta virt. eigenvalues -- 2.15024 2.15114 2.18637 2.19443 2.23022

Beta virt. eigenvalues -- 2.24187 2.24795 2.24967 2.25304 2.25824

Beta virt. eigenvalues -- 2.26339 2.26509 2.27092 2.27290 2.27361

Beta virt. eigenvalues -- 2.27659 2.27942 2.27945 2.28273 2.28411

Beta virt. eigenvalues -- 2.28443 2.28651 2.29291 2.30051 2.30067

Beta virt. eigenvalues -- 2.30488 2.30982 2.31238 2.31986 2.32773

Beta virt. eigenvalues -- 2.33307 2.33605 2.33800 2.33902 2.35668

Beta virt. eigenvalues -- 2.35858 2.36089 2.36562 2.37597 2.37644

Beta virt. eigenvalues -- 2.37850 2.38299 2.39845 2.40259 2.40680

Beta virt. eigenvalues -- 2.41156 2.41188 2.42197 2.44447 2.44922

Beta virt. eigenvalues -- 2.45920 2.46271 2.48580 2.48985 2.49646

Beta virt. eigenvalues -- 2.52584 2.52858 2.53998 2.54330 2.54383

Beta virt. eigenvalues -- 2.55382 2.57472 2.57694 2.58408 2.58897

Beta virt. eigenvalues -- 2.59105 2.59593 2.59820 2.60933 2.61252

Beta virt. eigenvalues -- 2.62792 2.63362 2.63686 2.64393 2.65452

Beta virt. eigenvalues -- 2.65465 2.66315 2.66338 2.66627 2.68825

Beta virt. eigenvalues -- 2.68952 2.70554 2.70869 2.70962 2.71315

Beta virt. eigenvalues -- 2.72218 2.73572 2.73672 2.74276 2.74938

Beta virt. eigenvalues -- 2.75124 2.76128 2.76153 2.78018 2.78066

Beta virt. eigenvalues -- 2.78418 2.78849 2.79432 2.79660 2.80080

Beta virt. eigenvalues -- 2.80765 2.83598 2.84330 2.84398 2.84411

Beta virt. eigenvalues -- 2.85479 2.86515 2.86795 2.87298 2.88222

Beta virt. eigenvalues -- 2.90484 2.91146 2.91319 2.91736 2.93080

Beta virt. eigenvalues -- 2.95820 2.96374 2.96637 2.98860 2.99722

Beta virt. eigenvalues -- 2.99861 3.00636 3.01649 3.03690 3.04486

Beta virt. eigenvalues -- 3.04823 3.05433 3.05960 3.06519 3.06742

Beta virt. eigenvalues -- 3.08377 3.08983 3.09391 3.09784 3.09884

Beta virt. eigenvalues -- 3.11422 3.11998 3.13196 3.13230 3.15052

Beta virt. eigenvalues -- 3.16472 3.16679 3.17824 3.18170 3.19065

Beta virt. eigenvalues -- 3.20654 3.21221 3.23356 3.25109 3.25141

Beta virt. eigenvalues -- 3.25883 3.26504 3.26737 3.27008 3.28401

Beta virt. eigenvalues -- 3.28910 3.30190 3.30364 3.30569 3.30802

Beta virt. eigenvalues -- 3.31157 3.31253 3.31324 3.31339 3.31862

Beta virt. eigenvalues -- 3.32196 3.32619 3.32944 3.33212 3.34090

Beta virt. eigenvalues -- 3.34307 3.34535 3.36048 3.36505 3.37422

Beta virt. eigenvalues -- 3.37958 3.37991 3.38785 3.40181 3.41164

Beta virt. eigenvalues -- 3.42806 3.43951 3.44128 3.46544 3.46560

Beta virt. eigenvalues -- 3.49735 3.51628 3.51891 3.52670 3.57721

Beta virt. eigenvalues -- 3.57747 3.58997 3.59097 3.59217 3.60878

Beta virt. eigenvalues -- 3.62425 3.63353 3.64518 3.66163 3.66261

Beta virt. eigenvalues -- 3.67509 3.72610 3.72844 3.73165 3.75722

Beta virt. eigenvalues -- 3.77707 3.78950 3.82481 3.82913 3.85043

Beta virt. eigenvalues -- 3.85938 3.89994 3.91921 3.92868 3.94273

Beta virt. eigenvalues -- 3.94524 3.94994 3.96568 3.96763 3.97009

Beta virt. eigenvalues -- 3.97269 3.99774 4.00311 4.04640 4.12158

Beta virt. eigenvalues -- 4.30923 4.32091 4.38310 4.42177 4.49322

Beta virt. eigenvalues -- 4.53385 4.56503 4.57452 4.65128 4.65389

Beta virt. eigenvalues -- 4.68736 4.70258 4.79237 4.79250 4.79259

Beta virt. eigenvalues -- 4.79276 5.10996 5.17152 5.18733 5.28804

Beta virt. eigenvalues -- 23.25460 23.28956 23.29063 23.30761 23.47445

Beta virt. eigenvalues -- 23.53834 23.55657 23.60974 23.76475 23.79081

Beta virt. eigenvalues -- 23.79467 23.81151 23.81350 23.81351 23.81620

Beta virt. eigenvalues -- 23.82372 23.86269 23.86976 23.87011 23.87625

Beta virt. eigenvalues -- 23.92345 23.93380 23.96599 23.97756 23.99910

Beta virt. eigenvalues -- 24.00035 24.01375 24.01663 24.05571 24.05704

Beta virt. eigenvalues -- 24.05753 24.05905 24.08353 24.08609 24.10098

Beta virt. eigenvalues -- 24.10197 24.13741 24.14001 24.14125 24.14664

Beta virt. eigenvalues -- 24.16229 24.16296 24.16300 24.16399 35.57998

Beta virt. eigenvalues -- 35.58894 35.65233 35.65764

Condensed to atoms (all electrons):

Atomic-Atomic Spin Densities.

Mulliken charges and spin densities:

1 2

1 C -0.277134 0.003729

2 C 0.317245 0.012012

3 N -0.711777 0.062206

4 C 0.317245 0.012012

5 C -0.277134 0.003729

6 C -0.121088 0.071136

7 C 0.162730 0.077249

8 N -0.491517 -0.027505

9 C 0.159599 0.077848

10 C -0.300253 0.063582

11 C -0.299130 0.064056

12 C -0.121088 0.071136

13 C 0.162730 0.077249

14 C -0.299130 0.064056

15 C -0.300253 0.063582

16 C 0.159599 0.077848

17 N -0.491517 -0.027505

18 C -0.115657 0.070992

19 C 0.314876 0.012015

20 C -0.277169 0.003728

21 C -0.277169 0.003728

22 C 0.314876 0.012015

23 N -0.709534 0.061937

24 C -0.115657 0.070992

25 C -0.085243 -0.009218

26 C -0.228219 0.011429

27 C -0.220330 -0.003572

28 C -0.227222 0.008735

29 C -0.222334 -0.001966

30 C -0.216932 0.005432

31 C -0.227222 0.008735

32 C -0.220330 -0.003572

33 C -0.228219 0.011429

34 C -0.085243 -0.009218

35 C -0.216932 0.005432

36 C -0.222334 -0.001966

37 C -0.084285 -0.009423

38 C -0.217081 0.005726

39 C -0.222484 -0.002133

40 C -0.227220 0.009160

41 C -0.220379 -0.003778

42 C -0.228697 0.011815

43 C -0.084285 -0.009423

44 C -0.217081 0.005726

45 C -0.222484 -0.002133

46 C -0.227220 0.009160

47 C -0.220379 -0.003778

48 C -0.228697 0.011815

49 H 0.241674 -0.000029

50 H 0.241674 -0.000029

51 H 0.213387 -0.003927

52 H 0.213500 -0.003956

53 H 0.213500 -0.003956

54 H 0.213387 -0.003927

55 H 0.241663 -0.000031

56 H 0.241663 -0.000031

57 H 0.224038 -0.000861

58 H 0.222652 0.000176

59 H 0.222266 -0.000489

60 H 0.222503 0.000280

61 H 0.221500 -0.000448

62 H 0.222266 -0.000489

63 H 0.222652 0.000176

64 H 0.224038 -0.000861

65 H 0.221500 -0.000448

66 H 0.222503 0.000280

67 H 0.221835 -0.000469

68 H 0.222521 0.000289

69 H 0.222269 -0.000512

70 H 0.222663 0.000182

71 H 0.224111 -0.000878

72 H 0.221835 -0.000469

73 H 0.222521 0.000289

74 H 0.222269 -0.000512

75 H 0.222663 0.000182

76 H 0.224111 -0.000878

77 H 0.401738 -0.002403

78 H 0.402253 -0.002499

Sum of Mulliken charges = -1.00000 1.00000

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

1 2

1 C -0.035460 0.003701

2 C 0.317245 0.012012

3 N -0.310039 0.059803

4 C 0.317245 0.012012

5 C -0.035460 0.003701

6 C -0.121088 0.071136

7 C 0.162730 0.077249

8 N -0.491517 -0.027505

9 C 0.159599 0.077848

10 C -0.086866 0.059655

11 C -0.085630 0.060100

12 C -0.121088 0.071136

13 C 0.162730 0.077249

14 C -0.085630 0.060100

15 C -0.086866 0.059655

16 C 0.159599 0.077848

17 N -0.491517 -0.027505

18 C -0.115657 0.070992

19 C 0.314876 0.012015

20 C -0.035505 0.003697

21 C -0.035505 0.003697

22 C 0.314876 0.012015

23 N -0.307281 0.059437

24 C -0.115657 0.070992

25 C -0.085243 -0.009218

26 C -0.004181 0.010569

27 C 0.002322 -0.003395

28 C -0.004955 0.008246

29 C 0.000169 -0.001687

30 C 0.004568 0.004984

31 C -0.004955 0.008246

32 C 0.002322 -0.003395

33 C -0.004181 0.010569

34 C -0.085243 -0.009218

35 C 0.004568 0.004984

36 C 0.000169 -0.001687

37 C -0.084285 -0.009423

38 C 0.004754 0.005257

39 C 0.000038 -0.001844

40 C -0.004951 0.008649

41 C 0.002284 -0.003596

42 C -0.004586 0.010937

43 C -0.084285 -0.009423

44 C 0.004754 0.005257

45 C 0.000038 -0.001844

46 C -0.004951 0.008649

47 C 0.002284 -0.003596

48 C -0.004586 0.010937

Electronic spatial extent (au): <R\*\*2>= 33256.2422

Charge= -1.0000 electrons

Dipole moment (field-independent basis, Debye):

X= -0.2953 Y= 0.0118 Z= 0.0000 Tot= 0.2955

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

XX= -281.5560 YY= -257.6087 ZZ= -289.5669

XY= -0.1438 XZ= -0.0000 YZ= -0.0000

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

XX= -5.3121 YY= 18.6351 ZZ= -13.3230

XY= -0.1438 XZ= -0.0000 YZ= -0.0000

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

XXX= -5.0464 YYY= 1.0945 ZZZ= -0.0000 XYY= 88.3580

XXY= -0.2171 XXZ= -0.0000 XZZ= -112.3940 YZZ= -0.6643

YYZ= -0.0000 XYZ= -0.0000

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

XXXX= -1022.0610 YYYY= -21376.0568 ZZZZ= -22471.5169 XXXY= -0.9871

XXXZ= -0.0000 YYYX= -5.5218 YYYZ= -0.0000 ZZZX= 0.0000

ZZZY= -0.0000 XXYY= -3963.5510 XXZZ= -4021.6739 YYZZ= -6445.0294

XXYZ= -0.0000 YYXZ= -0.0000 ZZXY= -3.3725

N-N= 5.359604218929D+03 E-N=-1.520414308746D+04 KE= 1.906691750895D+03

Symmetry A' KE= 1.008419543866D+03

Symmetry A" KE= 8.982722070289D+02

Isotropic Fermi Contact Couplings

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

1 C(13) -0.00057 -0.64024 -0.22845 -0.21356

2 C(13) -0.00357 -4.01572 -1.43291 -1.33950

3 N(14) 0.00837 2.70591 0.96554 0.90260

4 C(13) -0.00357 -4.01572 -1.43291 -1.33950

5 C(13) -0.00057 -0.64024 -0.22845 -0.21356

6 C(13) 0.00188 2.11207 0.75364 0.70451

7 C(13) 0.00154 1.73508 0.61912 0.57876

8 N(14) -0.00485 -1.56778 -0.55942 -0.52296

9 C(13) 0.00158 1.77670 0.63397 0.59264

10 C(13) -0.00008 -0.09056 -0.03231 -0.03021

11 C(13) -0.00004 -0.05019 -0.01791 -0.01674

12 C(13) 0.00188 2.11207 0.75364 0.70451

13 C(13) 0.00154 1.73508 0.61912 0.57876

14 C(13) -0.00004 -0.05019 -0.01791 -0.01674

15 C(13) -0.00008 -0.09056 -0.03231 -0.03021

16 C(13) 0.00158 1.77670 0.63397 0.59264

17 N(14) -0.00485 -1.56778 -0.55942 -0.52296

18 C(13) 0.00185 2.08065 0.74243 0.69403

19 C(13) -0.00354 -3.97483 -1.41832 -1.32586

20 C(13) -0.00058 -0.64684 -0.23081 -0.21576

21 C(13) -0.00058 -0.64684 -0.23081 -0.21576

22 C(13) -0.00354 -3.97483 -1.41832 -1.32586

23 N(14) 0.00831 2.68443 0.95787 0.89543

24 C(13) 0.00185 2.08065 0.74243 0.69403

25 C(13) -0.00281 -3.15645 -1.12630 -1.05288

26 C(13) 0.00275 3.08667 1.10140 1.02960

27 C(13) -0.00021 -0.23363 -0.08336 -0.07793

28 C(13) 0.00061 0.68111 0.24304 0.22719

29 C(13) -0.00046 -0.52120 -0.18598 -0.17385

30 C(13) 0.00080 0.89762 0.32029 0.29941

31 C(13) 0.00061 0.68111 0.24304 0.22719

32 C(13) -0.00021 -0.23363 -0.08336 -0.07793

33 C(13) 0.00275 3.08667 1.10140 1.02960

34 C(13) -0.00281 -3.15645 -1.12630 -1.05288

35 C(13) 0.00080 0.89762 0.32029 0.29941

36 C(13) -0.00046 -0.52120 -0.18598 -0.17385

37 C(13) -0.00278 -3.12501 -1.11508 -1.04239

38 C(13) 0.00078 0.87192 0.31112 0.29084

39 C(13) -0.00050 -0.55693 -0.19872 -0.18577

40 C(13) 0.00064 0.71879 0.25648 0.23976

41 C(13) -0.00025 -0.27774 -0.09910 -0.09264

42 C(13) 0.00274 3.08286 1.10004 1.02833

43 C(13) -0.00278 -3.12501 -1.11508 -1.04239

44 C(13) 0.00078 0.87192 0.31112 0.29084

45 C(13) -0.00050 -0.55693 -0.19872 -0.18577

46 C(13) 0.00064 0.71879 0.25648 0.23976

47 C(13) -0.00025 -0.27774 -0.09910 -0.09264

48 C(13) 0.00274 3.08286 1.10004 1.02833

49 H(1) -0.00006 -0.25960 -0.09263 -0.08659

50 H(1) -0.00006 -0.25960 -0.09263 -0.08659

51 H(1) -0.00116 -5.19551 -1.85389 -1.73304

52 H(1) -0.00117 -5.22445 -1.86421 -1.74269

53 H(1) -0.00117 -5.22445 -1.86421 -1.74269

54 H(1) -0.00116 -5.19551 -1.85389 -1.73304

55 H(1) -0.00006 -0.26081 -0.09306 -0.08700

56 H(1) -0.00006 -0.26081 -0.09306 -0.08700

57 H(1) -0.00015 -0.67044 -0.23923 -0.22363

58 H(1) 0.00005 0.21890 0.07811 0.07302

59 H(1) -0.00012 -0.54490 -0.19443 -0.18176

60 H(1) 0.00009 0.41967 0.14975 0.13999

61 H(1) -0.00005 -0.24336 -0.08684 -0.08117

62 H(1) -0.00012 -0.54490 -0.19443 -0.18176

63 H(1) 0.00005 0.21890 0.07811 0.07302

64 H(1) -0.00015 -0.67044 -0.23923 -0.22363

65 H(1) -0.00005 -0.24336 -0.08684 -0.08117

66 H(1) 0.00009 0.41967 0.14975 0.13999

67 H(1) -0.00006 -0.25672 -0.09161 -0.08563

68 H(1) 0.00010 0.43103 0.15380 0.14378

69 H(1) -0.00013 -0.57083 -0.20368 -0.19041

70 H(1) 0.00005 0.22364 0.07980 0.07460

71 H(1) -0.00016 -0.69399 -0.24763 -0.23149

72 H(1) -0.00006 -0.25672 -0.09161 -0.08563

73 H(1) 0.00010 0.43103 0.15380 0.14378

74 H(1) -0.00013 -0.57083 -0.20368 -0.19041

75 H(1) 0.00005 0.22364 0.07980 0.07460

76 H(1) -0.00016 -0.69399 -0.24763 -0.23149

77 H(1) -0.00111 -4.94389 -1.76410 -1.64911

78 H(1) -0.00112 -4.98600 -1.77913 -1.66315

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

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

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

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

1 Atom 0.002291 -0.000718 -0.001573

2 Atom 0.018902 -0.013175 -0.005727

3 Atom 0.153532 -0.073235 -0.080296

4 Atom 0.018902 -0.013175 -0.005727

5 Atom 0.002291 -0.000718 -0.001573

6 Atom 0.096540 -0.047551 -0.048989

7 Atom 0.093881 -0.050991 -0.042890

8 Atom -0.047300 0.027568 0.019732

9 Atom 0.094625 -0.051444 -0.043180

10 Atom 0.069553 -0.041880 -0.027673

11 Atom 0.070120 -0.042062 -0.028058

12 Atom 0.096540 -0.047551 -0.048989

13 Atom 0.093881 -0.050991 -0.042890

14 Atom 0.070120 -0.042062 -0.028058

15 Atom 0.069553 -0.041880 -0.027673

16 Atom 0.094625 -0.051444 -0.043180

17 Atom -0.047300 0.027568 0.019732

18 Atom 0.096670 -0.047556 -0.049114

19 Atom 0.018612 -0.012959 -0.005653

20 Atom 0.002157 -0.000579 -0.001577

21 Atom 0.002157 -0.000579 -0.001577

22 Atom 0.018612 -0.012959 -0.005653

23 Atom 0.150147 -0.070124 -0.080023

24 Atom 0.096670 -0.047556 -0.049114

25 Atom -0.003071 0.001229 0.001842

26 Atom -0.002661 0.005868 -0.003207

27 Atom -0.001266 0.001466 -0.000200

28 Atom 0.001406 -0.001226 -0.000180

29 Atom -0.000366 0.000899 -0.000534

30 Atom -0.005022 0.001041 0.003981

31 Atom 0.001406 -0.001226 -0.000180

32 Atom -0.001266 0.001466 -0.000200

33 Atom -0.002661 0.005868 -0.003207

34 Atom -0.003071 0.001229 0.001842

35 Atom -0.005022 0.001041 0.003981

36 Atom -0.000366 0.000899 -0.000534

37 Atom -0.003183 0.001263 0.001920

38 Atom -0.005127 0.001110 0.004017

39 Atom -0.000383 0.000910 -0.000527

40 Atom 0.001546 -0.001384 -0.000162

41 Atom -0.001296 0.001475 -0.000179

42 Atom -0.002479 0.005719 -0.003240

43 Atom -0.003183 0.001263 0.001920

44 Atom -0.005127 0.001110 0.004017

45 Atom -0.000383 0.000910 -0.000527

46 Atom 0.001546 -0.001384 -0.000162

47 Atom -0.001296 0.001475 -0.000179

48 Atom -0.002479 0.005719 -0.003240

49 Atom -0.001238 0.001020 0.000219

50 Atom -0.001238 0.001020 0.000219

51 Atom -0.001526 -0.002588 0.004114

52 Atom -0.001537 -0.002573 0.004110

53 Atom -0.001537 -0.002573 0.004110

54 Atom -0.001526 -0.002588 0.004114

55 Atom -0.001233 0.001011 0.000223

56 Atom -0.001233 0.001011 0.000223

57 Atom -0.000755 0.000929 -0.000174

58 Atom -0.000310 0.000374 -0.000063

59 Atom -0.000649 0.000334 0.000315

60 Atom -0.000378 0.000121 0.000257

61 Atom -0.000009 0.000094 -0.000085

62 Atom -0.000649 0.000334 0.000315

63 Atom -0.000310 0.000374 -0.000063

64 Atom -0.000755 0.000929 -0.000174

65 Atom -0.000009 0.000094 -0.000085

66 Atom -0.000378 0.000121 0.000257

67 Atom -0.000004 0.000113 -0.000109

68 Atom -0.000380 0.000124 0.000256

69 Atom -0.000660 0.000336 0.000324

70 Atom -0.000314 0.000370 -0.000057

71 Atom -0.000771 0.000924 -0.000153

72 Atom -0.000004 0.000113 -0.000109

73 Atom -0.000380 0.000124 0.000256

74 Atom -0.000660 0.000336 0.000324

75 Atom -0.000314 0.000370 -0.000057

76 Atom -0.000771 0.000924 -0.000153

77 Atom -0.003771 0.008096 -0.004325

78 Atom -0.003663 0.007944 -0.004281

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XY XZ YZ

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1 Atom -0.000977 0.000300 0.000541

2 Atom -0.004974 0.003350 -0.000349

3 Atom -0.053997 -0.000000 -0.000000

4 Atom -0.004974 -0.003350 0.000349

5 Atom -0.000977 -0.000300 -0.000541

6 Atom -0.018588 0.010774 -0.003738

7 Atom -0.006357 0.034277 -0.005156

8 Atom 0.000310 -0.017169 -0.000038

9 Atom 0.005455 0.034578 0.004938

10 Atom -0.000228 0.039198 -0.000411

11 Atom -0.000351 0.039041 0.000220

12 Atom -0.018588 -0.010774 0.003738

13 Atom -0.006357 -0.034277 0.005156

14 Atom -0.000351 -0.039041 -0.000220

15 Atom -0.000228 -0.039198 0.000411

16 Atom 0.005455 -0.034578 -0.004938

17 Atom 0.000310 0.017169 0.000038

18 Atom 0.018022 -0.009178 -0.003495

19 Atom 0.005359 0.003479 0.000393

20 Atom 0.001239 0.000203 -0.000560

21 Atom 0.001239 -0.000203 0.000560

22 Atom 0.005359 -0.003479 -0.000393

23 Atom 0.059533 0.000000 -0.000000

24 Atom 0.018022 0.009178 0.003495

25 Atom -0.002900 0.002458 0.003456

26 Atom 0.005704 -0.003623 -0.003800

27 Atom -0.001201 0.001881 0.002197

28 Atom 0.004695 -0.005503 -0.003095

29 Atom -0.000115 0.001280 0.001587

30 Atom 0.001816 0.000249 -0.005158

31 Atom 0.004695 0.005503 0.003095

32 Atom -0.001201 -0.001881 -0.002197

33 Atom 0.005704 0.003623 0.003800

34 Atom -0.002900 -0.002458 -0.003456

35 Atom 0.001816 -0.000249 0.005158

36 Atom -0.000115 -0.001280 -0.001587

37 Atom 0.003011 0.002553 -0.003535

38 Atom -0.001961 0.000066 0.005414

39 Atom 0.000188 0.001348 -0.001638

40 Atom -0.004880 -0.005803 0.003235

41 Atom 0.001271 0.001988 -0.002255

42 Atom -0.006041 -0.003858 0.003955

43 Atom 0.003011 -0.002553 0.003535

44 Atom -0.001961 -0.000066 -0.005414

45 Atom 0.000188 -0.001348 0.001638

46 Atom -0.004880 0.005803 -0.003235

47 Atom 0.001271 -0.001988 0.002255

48 Atom -0.006041 0.003858 -0.003955

49 Atom 0.000592 -0.000014 -0.000198

50 Atom 0.000592 0.000014 0.000198

51 Atom 0.001968 -0.001971 -0.005571

52 Atom -0.001977 -0.001942 0.005603

53 Atom -0.001977 0.001942 -0.005603

54 Atom 0.001968 0.001971 0.005571

55 Atom -0.000602 -0.000024 0.000194

56 Atom -0.000602 0.000024 -0.000194

57 Atom -0.001398 0.000105 0.000188

58 Atom -0.000201 0.000029 0.000436

59 Atom 0.000299 -0.000103 0.000831

60 Atom 0.000246 0.000347 0.000538

61 Atom 0.000905 0.001195 0.000936

62 Atom 0.000299 0.000103 -0.000831

63 Atom -0.000201 -0.000029 -0.000436

64 Atom -0.001398 -0.000105 -0.000188

65 Atom 0.000905 -0.001195 -0.000936

66 Atom 0.000246 -0.000347 -0.000538

67 Atom -0.000893 0.001192 -0.000949

68 Atom -0.000245 0.000348 -0.000541

69 Atom -0.000318 -0.000104 -0.000853

70 Atom 0.000194 0.000038 -0.000438

71 Atom 0.001384 0.000123 -0.000180

72 Atom -0.000893 -0.001192 0.000949

73 Atom -0.000245 -0.000348 0.000541

74 Atom -0.000318 0.000104 0.000853

75 Atom 0.000194 -0.000038 0.000438

76 Atom 0.001384 -0.000123 0.000180

77 Atom 0.002010 0.000000 -0.000000

78 Atom -0.002229 -0.000000 0.000000

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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 -0.0020 -0.263 -0.094 -0.088 -0.1759 -0.5060 0.8444

1 C(13) Bbb -0.0006 -0.084 -0.030 -0.028 0.2183 0.8163 0.5347

Bcc 0.0026 0.347 0.124 0.116 0.9599 -0.2784 0.0331

Baa -0.0139 -1.870 -0.667 -0.624 0.1517 0.9882 -0.0199

2 C(13) Bbb -0.0062 -0.827 -0.295 -0.276 -0.1248 0.0391 0.9914

Bcc 0.0201 2.696 0.962 0.899 0.9805 -0.1480 0.1292

Baa -0.0854 -3.295 -1.176 -1.099 0.2204 0.9754 0.0000

3 N(14) Bbb -0.0803 -3.097 -1.105 -1.033 -0.0000 -0.0000 1.0000

Bcc 0.1657 6.392 2.281 2.132 0.9754 -0.2204 -0.0000

Baa -0.0139 -1.870 -0.667 -0.624 0.1517 0.9882 0.0199

4 C(13) Bbb -0.0062 -0.827 -0.295 -0.276 0.1248 -0.0391 0.9914

Bcc 0.0201 2.696 0.962 0.899 0.9805 -0.1480 -0.1292

Baa -0.0020 -0.263 -0.094 -0.088 0.1759 0.5060 0.8444

5 C(13) Bbb -0.0006 -0.084 -0.030 -0.028 0.2183 0.8163 -0.5347

Bcc 0.0026 0.347 0.124 0.116 0.9599 -0.2784 -0.0331

Baa -0.0522 -7.007 -2.500 -2.337 0.0386 0.7143 0.6988

6 C(13) Bbb -0.0475 -6.377 -2.276 -2.127 -0.1420 -0.6883 0.7114

Bcc 0.0997 13.384 4.776 4.464 0.9891 -0.1267 0.0748

Baa -0.0547 -7.344 -2.620 -2.450 -0.1257 0.7233 0.6790

7 C(13) Bbb -0.0476 -6.390 -2.280 -2.131 -0.1997 -0.6889 0.6968

Bcc 0.1023 13.734 4.901 4.581 0.9718 -0.0481 0.2310

Baa -0.0514 -1.984 -0.708 -0.662 0.9721 -0.0037 0.2345

8 N(14) Bbb 0.0239 0.921 0.328 0.307 -0.2343 0.0296 0.9717

Bcc 0.0276 1.063 0.379 0.355 0.0105 0.9996 -0.0279

Baa -0.0551 -7.393 -2.638 -2.466 0.1302 0.7234 -0.6781

9 C(13) Bbb -0.0480 -6.440 -2.298 -2.148 -0.1955 0.6892 0.6977

Bcc 0.1031 13.833 4.936 4.614 0.9720 0.0417 0.2312

Baa -0.0421 -5.644 -2.014 -1.883 -0.1617 0.8702 0.4655

10 C(13) Bbb -0.0413 -5.546 -1.979 -1.850 -0.2909 -0.4927 0.8201

Bcc 0.0834 11.190 3.993 3.733 0.9430 -0.0028 0.3328

Baa -0.0422 -5.669 -2.023 -1.891 0.1666 0.8658 -0.4718

11 C(13) Bbb -0.0415 -5.569 -1.987 -1.858 -0.2845 0.5003 0.8178

Bcc 0.0838 11.239 4.010 3.749 0.9441 -0.0021 0.3296

Baa -0.0522 -7.007 -2.500 -2.337 0.0386 0.7143 -0.6988

12 C(13) Bbb -0.0475 -6.377 -2.276 -2.127 0.1420 0.6883 0.7114

Bcc 0.0997 13.384 4.776 4.464 0.9891 -0.1267 -0.0748

Baa -0.0547 -7.344 -2.620 -2.450 -0.1257 0.7233 -0.6790

13 C(13) Bbb -0.0476 -6.390 -2.280 -2.131 0.1997 0.6889 0.6968

Bcc 0.1023 13.734 4.901 4.581 0.9718 -0.0481 -0.2310

Baa -0.0422 -5.669 -2.023 -1.891 0.1666 0.8658 0.4718

14 C(13) Bbb -0.0415 -5.569 -1.987 -1.858 0.2845 -0.5003 0.8178

Bcc 0.0838 11.239 4.010 3.749 0.9441 -0.0021 -0.3296

Baa -0.0421 -5.644 -2.014 -1.883 -0.1617 0.8702 -0.4655

15 C(13) Bbb -0.0413 -5.546 -1.979 -1.850 0.2909 0.4927 0.8201

Bcc 0.0834 11.190 3.993 3.733 0.9430 -0.0028 -0.3328

Baa -0.0551 -7.393 -2.638 -2.466 0.1302 0.7234 0.6781

16 C(13) Bbb -0.0480 -6.440 -2.298 -2.148 0.1955 -0.6892 0.6977

Bcc 0.1031 13.833 4.936 4.614 0.9720 0.0417 -0.2312

Baa -0.0514 -1.984 -0.708 -0.662 0.9721 -0.0037 -0.2345

17 N(14) Bbb 0.0239 0.921 0.328 0.307 0.2343 -0.0296 0.9717

Bcc 0.0276 1.063 0.379 0.355 0.0105 0.9996 0.0279

Baa -0.0521 -6.990 -2.494 -2.332 -0.0428 0.7108 0.7020

18 C(13) Bbb -0.0474 -6.362 -2.270 -2.122 0.1318 -0.6925 0.7092

Bcc 0.0995 13.352 4.764 4.454 0.9904 0.1229 -0.0640

Baa -0.0138 -1.858 -0.663 -0.620 -0.1652 0.9860 0.0228

19 C(13) Bbb -0.0061 -0.822 -0.293 -0.274 -0.1296 -0.0447 0.9906

Bcc 0.0200 2.680 0.956 0.894 0.9777 0.1607 0.1352

Baa -0.0020 -0.264 -0.094 -0.088 -0.1949 0.5115 0.8369

20 C(13) Bbb -0.0007 -0.090 -0.032 -0.030 -0.3029 0.7802 -0.5474

Bcc 0.0026 0.353 0.126 0.118 0.9329 0.3601 -0.0029

Baa -0.0020 -0.264 -0.094 -0.088 0.1949 -0.5115 0.8369

21 C(13) Bbb -0.0007 -0.090 -0.032 -0.030 -0.3029 0.7802 0.5474

Bcc 0.0026 0.353 0.126 0.118 0.9329 0.3601 0.0029

Baa -0.0138 -1.858 -0.663 -0.620 -0.1652 0.9860 -0.0228

22 C(13) Bbb -0.0061 -0.822 -0.293 -0.274 0.1296 0.0447 0.9906

Bcc 0.0200 2.680 0.956 0.894 0.9777 0.1607 -0.1352

Baa -0.0852 -3.285 -1.172 -1.096 -0.2453 0.9695 0.0000

23 N(14) Bbb -0.0800 -3.086 -1.101 -1.029 0.0000 -0.0000 1.0000

Bcc 0.1652 6.372 2.274 2.125 0.9695 0.2453 0.0000

Baa -0.0521 -6.990 -2.494 -2.332 -0.0428 0.7108 -0.7020

24 C(13) Bbb -0.0474 -6.362 -2.270 -2.122 -0.1318 0.6925 0.7092

Bcc 0.0995 13.352 4.764 4.454 0.9904 0.1229 0.0640

Baa -0.0063 -0.851 -0.304 -0.284 0.7577 0.4879 -0.4334

25 C(13) Bbb 0.0013 0.179 0.064 0.060 0.6522 -0.5415 0.5305

Bcc 0.0050 0.672 0.240 0.224 -0.0241 0.6846 0.7285

Baa -0.0068 -0.906 -0.323 -0.302 0.7725 -0.1645 0.6133

26 C(13) Bbb -0.0038 -0.513 -0.183 -0.171 -0.4484 0.5425 0.7104

Bcc 0.0106 1.419 0.506 0.473 0.4496 0.8238 -0.3453

Baa -0.0037 -0.501 -0.179 -0.167 0.6707 0.4147 -0.6150

27 C(13) Bbb 0.0007 0.100 0.036 0.034 0.7413 -0.4028 0.5368

Bcc 0.0030 0.401 0.143 0.134 0.0251 0.8159 0.5776

Baa -0.0053 -0.715 -0.255 -0.239 0.7317 -0.4524 0.5098

28 C(13) Bbb -0.0038 -0.515 -0.184 -0.172 0.0108 0.7556 0.6550

Bcc 0.0092 1.231 0.439 0.411 0.6815 0.4737 -0.5577

Baa -0.0023 -0.305 -0.109 -0.102 -0.5287 -0.3954 0.7511

29 C(13) Bbb 0.0002 0.024 0.008 0.008 0.8040 -0.5171 0.2937

Bcc 0.0021 0.281 0.100 0.094 0.2722 0.7592 0.5912

Baa -0.0059 -0.794 -0.283 -0.265 0.8850 -0.4035 -0.2325

30 C(13) Bbb -0.0020 -0.271 -0.097 -0.091 0.4604 0.6827 0.5675

Bcc 0.0079 1.065 0.380 0.355 -0.0702 -0.6092 0.7899

Baa -0.0053 -0.715 -0.255 -0.239 0.7317 -0.4524 -0.5098

31 C(13) Bbb -0.0038 -0.515 -0.184 -0.172 0.0108 0.7556 -0.6550

Bcc 0.0092 1.231 0.439 0.411 0.6815 0.4737 0.5577

Baa -0.0037 -0.501 -0.179 -0.167 0.6707 0.4147 0.6150

32 C(13) Bbb 0.0007 0.100 0.036 0.034 0.7413 -0.4028 -0.5368

Bcc 0.0030 0.401 0.143 0.134 0.0251 0.8159 -0.5776

Baa -0.0068 -0.906 -0.323 -0.302 0.7725 -0.1645 -0.6133

33 C(13) Bbb -0.0038 -0.513 -0.183 -0.171 0.4484 -0.5425 0.7104

Bcc 0.0106 1.419 0.506 0.473 0.4496 0.8238 0.3453

Baa -0.0063 -0.851 -0.304 -0.284 0.7577 0.4879 0.4334

34 C(13) Bbb 0.0013 0.179 0.064 0.060 0.6522 -0.5415 -0.5305

Bcc 0.0050 0.672 0.240 0.224 0.0241 -0.6846 0.7285

Baa -0.0059 -0.794 -0.283 -0.265 0.8850 -0.4035 0.2325

35 C(13) Bbb -0.0020 -0.271 -0.097 -0.091 0.4604 0.6827 -0.5675

Bcc 0.0079 1.065 0.380 0.355 0.0702 0.6092 0.7899

Baa -0.0023 -0.305 -0.109 -0.102 0.5287 0.3954 0.7511

36 C(13) Bbb 0.0002 0.024 0.008 0.008 0.8040 -0.5171 -0.2937

Bcc 0.0021 0.281 0.100 0.094 0.2722 0.7592 -0.5912

Baa -0.0066 -0.881 -0.314 -0.294 0.7595 -0.4869 -0.4314

37 C(13) Bbb 0.0014 0.190 0.068 0.064 0.6502 0.5447 0.5297

Bcc 0.0051 0.690 0.246 0.230 -0.0230 -0.6828 0.7302

Baa -0.0061 -0.814 -0.290 -0.271 0.8819 0.4130 -0.2276

38 C(13) Bbb -0.0022 -0.296 -0.106 -0.099 -0.4636 0.6709 -0.5788

Bcc 0.0083 1.110 0.396 0.370 -0.0863 0.6159 0.7830

Baa -0.0024 -0.320 -0.114 -0.107 -0.5374 0.3999 0.7425

39 C(13) Bbb 0.0002 0.033 0.012 0.011 0.8013 0.5168 0.3016

Bcc 0.0021 0.287 0.102 0.096 -0.2631 0.7570 -0.5981

Baa -0.0056 -0.747 -0.267 -0.249 0.7292 0.4564 0.5099

40 C(13) Bbb -0.0041 -0.545 -0.195 -0.182 -0.0171 0.7570 -0.6531

Bcc 0.0096 1.292 0.461 0.431 0.6841 -0.4675 -0.5599

Baa -0.0039 -0.523 -0.186 -0.174 0.6721 -0.4162 -0.6124

41 C(13) Bbb 0.0008 0.113 0.040 0.038 0.7398 0.4114 0.5324

Bcc 0.0031 0.410 0.146 0.137 -0.0303 0.8109 -0.5844

Baa -0.0069 -0.931 -0.332 -0.311 0.7687 0.1746 0.6153

42 C(13) Bbb -0.0040 -0.535 -0.191 -0.178 -0.4370 -0.5591 0.7046

Bcc 0.0109 1.466 0.523 0.489 -0.4670 0.8105 0.3535

Baa -0.0066 -0.881 -0.314 -0.294 0.7595 -0.4869 0.4314

43 C(13) Bbb 0.0014 0.190 0.068 0.064 0.6502 0.5447 -0.5297

Bcc 0.0051 0.690 0.246 0.230 0.0230 0.6828 0.7302

Baa -0.0061 -0.814 -0.290 -0.271 0.8819 0.4130 0.2276

44 C(13) Bbb -0.0022 -0.296 -0.106 -0.099 -0.4636 0.6709 0.5788

Bcc 0.0083 1.110 0.396 0.370 0.0863 -0.6159 0.7830

Baa -0.0024 -0.320 -0.114 -0.107 0.5374 -0.3999 0.7425

45 C(13) Bbb 0.0002 0.033 0.012 0.011 0.8013 0.5168 -0.3016

Bcc 0.0021 0.287 0.102 0.096 -0.2631 0.7570 0.5981

Baa -0.0056 -0.747 -0.267 -0.249 0.7292 0.4564 -0.5099

46 C(13) Bbb -0.0041 -0.545 -0.195 -0.182 -0.0171 0.7570 0.6531

Bcc 0.0096 1.292 0.461 0.431 0.6841 -0.4675 0.5599

Baa -0.0039 -0.523 -0.186 -0.174 0.6721 -0.4162 0.6124

47 C(13) Bbb 0.0008 0.113 0.040 0.038 0.7398 0.4114 -0.5324

Bcc 0.0031 0.410 0.146 0.137 -0.0303 0.8109 0.5844

Baa -0.0069 -0.931 -0.332 -0.311 0.7687 0.1746 -0.6153

48 C(13) Bbb -0.0040 -0.535 -0.191 -0.178 0.4370 0.5591 0.7046

Bcc 0.0109 1.466 0.523 0.489 -0.4670 0.8105 -0.3535

Baa -0.0014 -0.739 -0.264 -0.247 0.9704 -0.2407 -0.0215

49 H(1) Bbb 0.0002 0.096 0.034 0.032 0.0674 0.1840 0.9806

Bcc 0.0012 0.643 0.229 0.214 0.2321 0.9530 -0.1948

Baa -0.0014 -0.739 -0.264 -0.247 0.9704 -0.2407 0.0215

50 H(1) Bbb 0.0002 0.096 0.034 0.032 -0.0674 -0.1840 0.9806

Bcc 0.0012 0.643 0.229 0.214 0.2321 0.9530 0.1948

Baa -0.0059 -3.139 -1.120 -1.047 -0.1913 0.8729 0.4488

51 H(1) Bbb -0.0021 -1.141 -0.407 -0.381 0.9432 0.0369 0.3302

Bcc 0.0080 4.280 1.527 1.428 -0.2717 -0.4864 0.8304

Baa -0.0059 -3.151 -1.124 -1.051 0.1944 0.8717 -0.4499

52 H(1) Bbb -0.0021 -1.137 -0.406 -0.379 0.9433 -0.0402 0.3296

Bcc 0.0080 4.288 1.530 1.430 -0.2692 0.4885 0.8300

Baa -0.0059 -3.151 -1.124 -1.051 0.1944 0.8717 0.4499

53 H(1) Bbb -0.0021 -1.137 -0.406 -0.379 0.9433 -0.0402 -0.3296

Bcc 0.0080 4.288 1.530 1.430 0.2692 -0.4885 0.8300

Baa -0.0059 -3.139 -1.120 -1.047 -0.1913 0.8729 -0.4488

54 H(1) Bbb -0.0021 -1.141 -0.407 -0.381 0.9432 0.0369 -0.3302

Bcc 0.0080 4.280 1.527 1.428 0.2717 0.4864 0.8304

Baa -0.0014 -0.739 -0.264 -0.246 0.9695 0.2448 -0.0149

55 H(1) Bbb 0.0002 0.098 0.035 0.033 0.0618 -0.1852 0.9808

Bcc 0.0012 0.640 0.229 0.214 -0.2373 0.9517 0.1946

Baa -0.0014 -0.739 -0.264 -0.246 0.9695 0.2448 0.0149

56 H(1) Bbb 0.0002 0.098 0.035 0.033 -0.0618 0.1852 0.9808

Bcc 0.0012 0.640 0.229 0.214 -0.2373 0.9517 -0.1946

Baa -0.0016 -0.837 -0.299 -0.279 0.8609 0.4916 -0.1313

57 H(1) Bbb -0.0002 -0.084 -0.030 -0.028 0.1434 0.0131 0.9896

Bcc 0.0017 0.921 0.329 0.307 -0.4882 0.8707 0.0593

Baa -0.0005 -0.247 -0.088 -0.082 0.7035 0.4539 -0.5469

58 H(1) Bbb -0.0002 -0.110 -0.039 -0.037 0.6925 -0.2649 0.6710

Bcc 0.0007 0.356 0.127 0.119 -0.1597 0.8507 0.5007

Baa -0.0009 -0.467 -0.167 -0.156 0.7921 -0.4663 0.3938

59 H(1) Bbb -0.0003 -0.155 -0.055 -0.052 -0.6052 -0.5164 0.6059

Bcc 0.0012 0.622 0.222 0.208 0.0792 0.7183 0.6912

Baa -0.0005 -0.283 -0.101 -0.094 0.9223 -0.0302 -0.3852

60 H(1) Bbb -0.0003 -0.183 -0.065 -0.061 -0.2162 0.7859 -0.5793

Bcc 0.0009 0.467 0.166 0.156 0.3202 0.6176 0.7183

Baa -0.0012 -0.664 -0.237 -0.222 -0.6675 -0.0670 0.7416

61 H(1) Bbb -0.0008 -0.416 -0.149 -0.139 -0.4535 0.8265 -0.3335

Bcc 0.0020 1.081 0.386 0.361 0.5906 0.5589 0.5821

Baa -0.0009 -0.467 -0.167 -0.156 0.7921 -0.4663 -0.3938

62 H(1) Bbb -0.0003 -0.155 -0.055 -0.052 0.6052 0.5164 0.6059

Bcc 0.0012 0.622 0.222 0.208 0.0792 0.7183 -0.6912

Baa -0.0005 -0.247 -0.088 -0.082 0.7035 0.4539 0.5469

63 H(1) Bbb -0.0002 -0.110 -0.039 -0.037 0.6925 -0.2649 -0.6710

Bcc 0.0007 0.356 0.127 0.119 -0.1597 0.8507 -0.5007

Baa -0.0016 -0.837 -0.299 -0.279 0.8609 0.4916 0.1313

64 H(1) Bbb -0.0002 -0.084 -0.030 -0.028 -0.1434 -0.0131 0.9896

Bcc 0.0017 0.921 0.329 0.307 -0.4882 0.8707 -0.0593

Baa -0.0012 -0.664 -0.237 -0.222 0.6675 0.0670 0.7416

65 H(1) Bbb -0.0008 -0.416 -0.149 -0.139 -0.4535 0.8265 0.3335

Bcc 0.0020 1.081 0.386 0.361 0.5906 0.5589 -0.5821

Baa -0.0005 -0.283 -0.101 -0.094 0.9223 -0.0302 0.3852

66 H(1) Bbb -0.0003 -0.183 -0.065 -0.061 -0.2162 0.7859 0.5793

Bcc 0.0009 0.467 0.166 0.156 -0.3202 -0.6176 0.7183

Baa -0.0013 -0.670 -0.239 -0.224 -0.6463 0.1027 0.7562

67 H(1) Bbb -0.0008 -0.409 -0.146 -0.137 0.4854 0.8199 0.3035

Bcc 0.0020 1.080 0.385 0.360 0.5888 -0.5632 0.5797

Baa -0.0005 -0.285 -0.102 -0.095 0.9201 0.0213 -0.3911

68 H(1) Bbb -0.0003 -0.184 -0.066 -0.061 0.2268 0.7850 0.5764

Bcc 0.0009 0.469 0.167 0.156 0.3193 -0.6191 0.7175

Baa -0.0009 -0.482 -0.172 -0.161 0.7869 0.4736 0.3955

69 H(1) Bbb -0.0003 -0.156 -0.056 -0.052 0.6113 -0.5112 -0.6042

Bcc 0.0012 0.638 0.228 0.213 -0.0840 0.7172 -0.6918

Baa -0.0005 -0.249 -0.089 -0.083 0.7066 -0.4497 -0.5463

70 H(1) Bbb -0.0002 -0.107 -0.038 -0.036 0.6919 0.2775 0.6665

Bcc 0.0007 0.355 0.127 0.119 0.1482 0.8490 -0.5072

Baa -0.0016 -0.839 -0.299 -0.280 0.8623 -0.4876 -0.1364

71 H(1) Bbb -0.0001 -0.070 -0.025 -0.023 0.1447 -0.0207 0.9893

Bcc 0.0017 0.909 0.324 0.303 0.4852 0.8728 -0.0527

Baa -0.0013 -0.670 -0.239 -0.224 0.6463 -0.1027 0.7562

72 H(1) Bbb -0.0008 -0.409 -0.146 -0.137 0.4854 0.8199 -0.3035

Bcc 0.0020 1.080 0.385 0.360 0.5888 -0.5632 -0.5797

Baa -0.0005 -0.285 -0.102 -0.095 0.9201 0.0213 0.3911

73 H(1) Bbb -0.0003 -0.184 -0.066 -0.061 0.2268 0.7850 -0.5764

Bcc 0.0009 0.469 0.167 0.156 -0.3193 0.6191 0.7175

Baa -0.0009 -0.482 -0.172 -0.161 0.7869 0.4736 -0.3955

74 H(1) Bbb -0.0003 -0.156 -0.056 -0.052 0.6113 -0.5112 0.6042

Bcc 0.0012 0.638 0.228 0.213 -0.0840 0.7172 0.6918

Baa -0.0005 -0.249 -0.089 -0.083 0.7066 -0.4497 0.5463

75 H(1) Bbb -0.0002 -0.107 -0.038 -0.036 0.6919 0.2775 -0.6665

Bcc 0.0007 0.355 0.127 0.119 0.1482 0.8490 0.5072

Baa -0.0016 -0.839 -0.299 -0.280 0.8623 -0.4876 0.1364

76 H(1) Bbb -0.0001 -0.070 -0.025 -0.023 -0.1447 0.0207 0.9893

Bcc 0.0017 0.909 0.324 0.303 0.4852 0.8728 0.0527

Baa -0.0043 -2.307 -0.823 -0.770 -0.0000 0.0000 1.0000

77 H(1) Bbb -0.0041 -2.189 -0.781 -0.730 0.9867 -0.1626 0.0000

Bcc 0.0084 4.496 1.604 1.500 0.1626 0.9867 -0.0000

Baa -0.0043 -2.284 -0.815 -0.762 0.0000 0.0000 1.0000

78 H(1) Bbb -0.0041 -2.175 -0.776 -0.726 0.9832 0.1823 -0.0000

Bcc 0.0084 4.459 1.591 1.487 -0.1823 0.9832 0.0000

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

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Sun Aug 18 13:50:54 2019, MaxMem= 2013265920 cpu: 33.9

(Enter /home/kira/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 = 186

Leave Link 701 at Sun Aug 18 13:51:12 2019, MaxMem= 2013265920 cpu: 138.7

(Enter /home/kira/g09/l702.exe)

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

Leave Link 702 at Sun Aug 18 13:51:12 2019, MaxMem= 2013265920 cpu: 0.1

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 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= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

Petite list used in FoFCou.

Leave Link 703 at Sun Aug 18 13:52:27 2019, MaxMem= 2013265920 cpu: 604.8

(Enter /home/kira/g09/l716.exe)

Dipole =-1.16160432D-01 4.65110968D-03-3.35731443D-13

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.002058161 -0.000360336 -0.003972418

2 6 -0.005228470 0.001615229 0.015146745

3 7 -0.002232238 -0.000609502 -0.000000000

4 6 -0.005228469 0.001615229 -0.015146745

5 6 0.002058161 -0.000360336 0.003972418

6 6 0.000816138 -0.000017545 0.006541886

7 6 0.004824588 -0.001431719 0.005063129

8 7 0.000076612 0.001796113 -0.001432372

9 6 -0.004965315 -0.001417136 0.005035734

10 6 0.000771470 0.000433932 -0.001515373

11 6 -0.000766443 0.000431449 -0.001522783

12 6 0.000816138 -0.000017545 -0.006541886

13 6 0.004824588 -0.001431719 -0.005063129

14 6 -0.000766443 0.000431449 0.001522783

15 6 0.000771470 0.000433932 0.001515373

16 6 -0.004965315 -0.001417136 -0.005035734

17 7 0.000076612 0.001796113 0.001432372

18 6 -0.000706733 0.000071266 -0.006537867

19 6 0.005232625 0.001505509 0.015124716

20 6 -0.002067582 -0.000320609 -0.003972750

21 6 -0.002067582 -0.000320609 0.003972750

22 6 0.005232626 0.001505509 -0.015124716

23 7 0.002145713 -0.000568008 0.000000000

24 6 -0.000706733 0.000071266 0.006537867

25 6 -0.000544152 -0.000276906 0.000475458

26 6 -0.000631093 -0.000693574 -0.002051443

27 6 0.000688941 -0.000390543 -0.000056810

28 6 0.000622620 0.000005878 -0.000596051

29 6 -0.000008293 0.000226945 -0.000714516

30 6 0.002199930 0.000767121 0.000354392

31 6 0.000622620 0.000005878 0.000596051

32 6 0.000688941 -0.000390543 0.000056810

33 6 -0.000631093 -0.000693574 0.002051443

34 6 -0.000544152 -0.000276906 -0.000475458

35 6 0.002199930 0.000767121 -0.000354392

36 6 -0.000008293 0.000226945 0.000714516

37 6 0.000507752 -0.000267790 0.000449465

38 6 -0.002207808 0.000758425 0.000371186

39 6 -0.000004772 0.000239923 -0.000711082

40 6 -0.000638202 0.000009076 -0.000603611

41 6 -0.000689573 -0.000418489 -0.000071544

42 6 0.000666586 -0.000684230 -0.002052570

43 6 0.000507752 -0.000267790 -0.000449465

44 6 -0.002207808 0.000758425 -0.000371186

45 6 -0.000004772 0.000239923 0.000711082

46 6 -0.000638202 0.000009076 0.000603611

47 6 -0.000689573 -0.000418489 0.000071544

48 6 0.000666586 -0.000684230 0.002052570

49 1 0.000252987 0.000027116 0.000248446

50 1 0.000252987 0.000027116 -0.000248446

51 1 -0.000275775 0.000060410 -0.000343805

52 1 0.000277705 0.000057622 -0.000344266

53 1 0.000277705 0.000057622 0.000344266

54 1 -0.000275775 0.000060410 0.000343805

55 1 -0.000253530 0.000026862 0.000249825

56 1 -0.000253530 0.000026862 -0.000249825

57 1 -0.000164701 -0.000016575 0.000090730

58 1 0.000374922 0.000087805 -0.000150893

59 1 0.000144656 -0.000008358 -0.000152139

60 1 0.000144577 -0.000116101 -0.000371559

61 1 -0.000087139 -0.000061514 0.000150586

62 1 0.000144656 -0.000008358 0.000152139

63 1 0.000374922 0.000087805 0.000150893

64 1 -0.000164701 -0.000016575 -0.000090730

65 1 -0.000087139 -0.000061514 -0.000150586

66 1 0.000144577 -0.000116101 0.000371559

67 1 0.000090721 -0.000056685 0.000153434

68 1 -0.000144293 -0.000118062 -0.000372999

69 1 -0.000145928 -0.000005892 -0.000154257

70 1 -0.000377986 0.000088717 -0.000149305

71 1 0.000173655 -0.000015327 0.000096267

72 1 0.000090721 -0.000056685 -0.000153434

73 1 -0.000144293 -0.000118062 0.000372999

74 1 -0.000145928 -0.000005892 0.000154257

75 1 -0.000377986 0.000088717 0.000149305

76 1 0.000173655 -0.000015327 -0.000096267

77 1 0.000908159 -0.000840191 0.000000000

78 1 -0.000855348 -0.001046312 -0.000000000

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

Cartesian Forces: Max 0.015146745 RMS 0.002605114

Leave Link 716 at Sun Aug 18 13:52:27 2019, MaxMem= 2013265920 cpu: 0.2

(Enter /home/kira/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

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

Internal Forces: Max 0.006821160 RMS 0.001297908

Search for a local minimum.

Step number 1 out of a maximum of 452

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

RMS Force = .12979D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Second derivative matrix not updated -- first step.

ITU= 0

Eigenvalues --- 0.00983 0.00983 0.00988 0.00988 0.01615

Eigenvalues --- 0.01615 0.01621 0.01653 0.01661 0.01668

Eigenvalues --- 0.01725 0.01725 0.01725 0.01725 0.01738

Eigenvalues --- 0.01751 0.01754 0.01801 0.01804 0.01824

Eigenvalues --- 0.01835 0.01855 0.01866 0.01868 0.01894

Eigenvalues --- 0.01904 0.01931 0.01944 0.01946 0.01980

Eigenvalues --- 0.01981 0.02014 0.02020 0.02026 0.02051

Eigenvalues --- 0.02068 0.02068 0.02070 0.02070 0.02086

Eigenvalues --- 0.02098 0.02109 0.02119 0.02119 0.02120

Eigenvalues --- 0.02120 0.02130 0.02132 0.02132 0.02133

Eigenvalues --- 0.02133 0.02137 0.02160 0.02160 0.02160

Eigenvalues --- 0.02160 0.02162 0.02162 0.02162 0.02162

Eigenvalues --- 0.02173 0.02173 0.02173 0.02173 0.02181

Eigenvalues --- 0.02181 0.02181 0.02181 0.02186 0.02186

Eigenvalues --- 0.02187 0.02187 0.02216 0.02220 0.02297

Eigenvalues --- 0.15969 0.15986 0.15989 0.15992 0.15994

Eigenvalues --- 0.15996 0.15996 0.15996 0.15996 0.15996

Eigenvalues --- 0.15997 0.15997 0.15997 0.15997 0.15997

Eigenvalues --- 0.15997 0.15998 0.15998 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.21999 0.21999 0.21999 0.21999 0.22000

Eigenvalues --- 0.22000 0.22000 0.22000 0.22729 0.22770

Eigenvalues --- 0.22800 0.22818 0.23472 0.23472 0.23473

Eigenvalues --- 0.23473 0.23531 0.23546 0.23751 0.24525

Eigenvalues --- 0.24733 0.24738 0.24875 0.24987 0.24991

Eigenvalues --- 0.24991 0.24997 0.24999 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.34159 0.34159 0.34206

Eigenvalues --- 0.34206 0.35413 0.35413 0.35413 0.35413

Eigenvalues --- 0.35415 0.35415 0.35416 0.35416 0.35416

Eigenvalues --- 0.35416 0.35416 0.35416 0.35506 0.35506

Eigenvalues --- 0.35508 0.35508 0.35542 0.35542 0.35547

Eigenvalues --- 0.35547 0.36056 0.36056 0.36058 0.36058

Eigenvalues --- 0.36250 0.36250 0.36251 0.36251 0.37073

Eigenvalues --- 0.37111 0.37229 0.37262 0.39153 0.39274

Eigenvalues --- 0.39734 0.40111 0.40225 0.40408 0.40439

Eigenvalues --- 0.40472 0.41759 0.41759 0.41774 0.41774

Eigenvalues --- 0.42117 0.42117 0.42121 0.42121 0.43225

Eigenvalues --- 0.44089 0.44648 0.45378 0.45567 0.45567

Eigenvalues --- 0.45584 0.45584 0.45642 0.45757 0.45796

Eigenvalues --- 0.45930 0.45930 0.45936 0.45942 0.45942

Eigenvalues --- 0.45953 0.45967 0.46660 0.46660 0.46661

Eigenvalues --- 0.46661 0.47073 0.47073 0.47085 0.47085

Eigenvalues --- 0.48153 0.48251 0.49301 0.49400 0.49962

Eigenvalues --- 0.50219 0.50788 0.50843

RFO step: Lambda=-3.05414518D-03 EMin= 9.82638911D-03

Linear search not attempted -- first point.

Iteration 1 RMS(Cart)= 0.05778395 RMS(Int)= 0.00080142

Iteration 2 RMS(Cart)= 0.00132633 RMS(Int)= 0.00005472

Iteration 3 RMS(Cart)= 0.00000096 RMS(Int)= 0.00005472

ITry= 1 IFail=0 DXMaxC= 2.17D-01 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.24D-08 for atom 74.

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

(Linear) (Quad) (Total)

R1 2.71383 0.00327 0.00000 0.00760 0.00762 2.72145

R2 2.58226 -0.00035 0.00000 -0.00187 -0.00180 2.58045

R3 2.03692 0.00034 0.00000 0.00093 0.00093 2.03784

R4 2.60481 0.00505 0.00000 0.01119 0.01113 2.61595

R5 2.64159 -0.00682 0.00000 -0.01475 -0.01474 2.62685

R6 2.60481 0.00505 0.00000 0.01119 0.01113 2.61595

R7 1.91107 -0.00103 0.00000 -0.00223 -0.00223 1.90884

R8 2.71383 0.00327 0.00000 0.00760 0.00762 2.72145

R9 2.64159 -0.00682 0.00000 -0.01475 -0.01474 2.62685

R10 2.03692 0.00034 0.00000 0.00093 0.00093 2.03784

R11 2.70900 -0.00074 0.00000 -0.00182 -0.00182 2.70718

R12 2.80363 0.00409 0.00000 0.01186 0.01186 2.81549

R13 2.59048 0.00203 0.00000 0.00454 0.00448 2.59496

R14 2.70765 0.00229 0.00000 0.00534 0.00536 2.71301

R15 2.59036 0.00210 0.00000 0.00467 0.00461 2.59497

R16 2.70749 0.00229 0.00000 0.00535 0.00537 2.71286

R17 2.70947 -0.00079 0.00000 -0.00193 -0.00193 2.70754

R18 2.60227 0.00107 0.00000 0.00141 0.00148 2.60375

R19 2.03995 0.00044 0.00000 0.00122 0.00122 2.04117

R20 2.03991 0.00044 0.00000 0.00122 0.00122 2.04114

R21 2.70900 -0.00074 0.00000 -0.00182 -0.00182 2.70718

R22 2.80363 0.00409 0.00000 0.01186 0.01186 2.81549

R23 2.70765 0.00229 0.00000 0.00534 0.00536 2.71301

R24 2.59048 0.00203 0.00000 0.00454 0.00448 2.59496

R25 2.60227 0.00107 0.00000 0.00141 0.00148 2.60375

R26 2.03991 0.00044 0.00000 0.00122 0.00122 2.04114

R27 2.70749 0.00229 0.00000 0.00535 0.00537 2.71286

R28 2.03995 0.00044 0.00000 0.00122 0.00122 2.04117

R29 2.59036 0.00210 0.00000 0.00467 0.00461 2.59497

R30 2.70947 -0.00079 0.00000 -0.00193 -0.00193 2.70754

R31 2.64179 -0.00679 0.00000 -0.01467 -0.01467 2.62711

R32 2.80284 0.00413 0.00000 0.01196 0.01196 2.81480

R33 2.71366 0.00327 0.00000 0.00760 0.00762 2.72128

R34 2.60463 0.00501 0.00000 0.01110 0.01104 2.61568

R35 2.58231 -0.00034 0.00000 -0.00184 -0.00177 2.58054

R36 2.03692 0.00034 0.00000 0.00093 0.00093 2.03785

R37 2.71366 0.00327 0.00000 0.00760 0.00762 2.72128

R38 2.03692 0.00034 0.00000 0.00093 0.00093 2.03785

R39 2.60463 0.00501 0.00000 0.01110 0.01104 2.61568

R40 2.64179 -0.00679 0.00000 -0.01467 -0.01467 2.62711

R41 1.91062 -0.00103 0.00000 -0.00224 -0.00224 1.90838

R42 2.80284 0.00413 0.00000 0.01196 0.01196 2.81480

R43 2.64992 0.00033 0.00000 0.00069 0.00069 2.65061

R44 2.65128 0.00049 0.00000 0.00104 0.00104 2.65232

R45 2.63102 0.00144 0.00000 0.00305 0.00305 2.63407

R46 2.04861 0.00004 0.00000 0.00013 0.00013 2.04873

R47 2.63393 -0.00025 0.00000 -0.00049 -0.00049 2.63344

R48 2.05006 0.00034 0.00000 0.00095 0.00095 2.05101

R49 2.63664 -0.00022 0.00000 -0.00042 -0.00042 2.63622

R50 2.05006 0.00021 0.00000 0.00059 0.00059 2.05064

R51 2.62811 0.00139 0.00000 0.00294 0.00294 2.63105

R52 2.05010 0.00034 0.00000 0.00095 0.00095 2.05105

R53 2.04804 0.00010 0.00000 0.00029 0.00029 2.04833

R54 2.63393 -0.00025 0.00000 -0.00049 -0.00049 2.63344

R55 2.63664 -0.00022 0.00000 -0.00042 -0.00042 2.63622

R56 2.05006 0.00021 0.00000 0.00059 0.00059 2.05064

R57 2.63102 0.00144 0.00000 0.00305 0.00305 2.63407

R58 2.05006 0.00034 0.00000 0.00095 0.00095 2.05101

R59 2.64992 0.00033 0.00000 0.00069 0.00069 2.65061

R60 2.04861 0.00004 0.00000 0.00013 0.00013 2.04873

R61 2.65128 0.00049 0.00000 0.00104 0.00104 2.65232

R62 2.62811 0.00139 0.00000 0.00294 0.00294 2.63105

R63 2.04804 0.00010 0.00000 0.00029 0.00029 2.04833

R64 2.05010 0.00034 0.00000 0.00095 0.00095 2.05105

R65 2.65163 0.00047 0.00000 0.00100 0.00100 2.65264

R66 2.65020 0.00031 0.00000 0.00064 0.00064 2.65084

R67 2.62794 0.00141 0.00000 0.00298 0.00298 2.63092

R68 2.04796 0.00010 0.00000 0.00029 0.00029 2.04825

R69 2.63669 -0.00022 0.00000 -0.00042 -0.00042 2.63627

R70 2.05010 0.00034 0.00000 0.00096 0.00096 2.05105

R71 2.63394 -0.00026 0.00000 -0.00051 -0.00051 2.63342

R72 2.05005 0.00021 0.00000 0.00059 0.00059 2.05064

R73 2.63094 0.00146 0.00000 0.00309 0.00309 2.63403

R74 2.05005 0.00034 0.00000 0.00096 0.00096 2.05101

R75 2.04858 0.00005 0.00000 0.00013 0.00013 2.04871

R76 2.65163 0.00047 0.00000 0.00100 0.00100 2.65264

R77 2.65020 0.00031 0.00000 0.00064 0.00064 2.65084

R78 2.62794 0.00141 0.00000 0.00298 0.00298 2.63092

R79 2.04796 0.00010 0.00000 0.00029 0.00029 2.04825

R80 2.63669 -0.00022 0.00000 -0.00042 -0.00042 2.63627

R81 2.05010 0.00034 0.00000 0.00096 0.00096 2.05105

R82 2.63394 -0.00026 0.00000 -0.00051 -0.00051 2.63342

R83 2.05005 0.00021 0.00000 0.00059 0.00059 2.05064

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A2 2.17810 -0.00098 0.00000 -0.00324 -0.00323 2.17487

A3 2.21516 -0.00087 0.00000 -0.00257 -0.00255 2.21261

A4 1.85690 -0.00284 0.00000 -0.01087 -0.01089 1.84601

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A6 2.20551 0.00182 0.00000 0.00970 0.00949 2.21499

A7 1.93092 0.00197 0.00000 0.00985 0.00990 1.94082

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A16 2.18918 -0.00219 0.00000 -0.00510 -0.00537 2.18381

A17 2.04466 0.00115 0.00000 0.00277 0.00290 2.04757

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A19 2.17593 0.00278 0.00000 0.01366 0.01344 2.18937

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D9 -0.03403 -0.00011 0.00000 -0.00577 -0.00576 -0.03979

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D137 0.00646 -0.00016 0.00000 -0.00614 -0.00611 0.00035

D138 -3.13561 0.00000 0.00000 0.00059 0.00060 -3.13501

D139 -3.13317 -0.00016 0.00000 -0.00628 -0.00625 -3.13942

D140 0.00795 0.00000 0.00000 0.00044 0.00045 0.00840

D141 -0.01784 0.00029 0.00000 0.01204 0.01205 -0.00578

D142 -3.13887 0.00015 0.00000 0.00621 0.00621 -3.13266

D143 3.12423 0.00012 0.00000 0.00535 0.00537 3.12959

D144 0.00319 -0.00002 0.00000 -0.00048 -0.00047 0.00272

D145 -0.00773 0.00016 0.00000 0.00633 0.00630 -0.00144

D146 3.13175 -0.00000 0.00000 -0.00011 -0.00013 3.13163

D147 3.13582 0.00016 0.00000 0.00618 0.00615 -3.14121

D148 -0.00788 -0.00000 0.00000 -0.00026 -0.00027 -0.00815

D149 -0.00646 0.00016 0.00000 0.00614 0.00611 -0.00035

D150 3.13561 -0.00000 0.00000 -0.00059 -0.00060 3.13501

D151 3.13317 0.00016 0.00000 0.00628 0.00625 3.13942

D152 -0.00795 -0.00000 0.00000 -0.00044 -0.00045 -0.00840

D153 0.01068 -0.00032 0.00000 -0.01283 -0.01285 -0.00217

D154 3.13107 -0.00012 0.00000 -0.00485 -0.00485 3.12622

D155 -3.12882 -0.00015 0.00000 -0.00642 -0.00644 -3.13526

D156 -0.00843 0.00004 0.00000 0.00157 0.00156 -0.00687

D157 3.13843 0.00018 0.00000 0.00730 0.00730 -3.13745

D158 0.00054 0.00017 0.00000 0.00683 0.00683 0.00737

D159 0.01793 -0.00002 0.00000 -0.00067 -0.00067 0.01726

D160 -3.11996 -0.00003 0.00000 -0.00114 -0.00115 -3.12110

D161 3.13050 0.00013 0.00000 0.00513 0.00513 3.13563

D162 0.00934 -0.00001 0.00000 -0.00068 -0.00069 0.00866

D163 -0.01477 0.00014 0.00000 0.00560 0.00560 -0.00917

D164 -3.13593 0.00000 0.00000 -0.00021 -0.00022 -3.13614

D165 0.01784 -0.00029 0.00000 -0.01204 -0.01205 0.00578

D166 -3.12423 -0.00012 0.00000 -0.00535 -0.00537 -3.12959

D167 3.13887 -0.00015 0.00000 -0.00621 -0.00621 3.13266

D168 -0.00319 0.00002 0.00000 0.00048 0.00047 -0.00272

D169 3.12808 0.00013 0.00000 0.00516 0.00516 3.13324

D170 0.00793 -0.00001 0.00000 -0.00071 -0.00072 0.00721

D171 -0.01490 0.00014 0.00000 0.00555 0.00555 -0.00935

D172 -3.13505 -0.00000 0.00000 -0.00033 -0.00033 -3.13538

D173 3.14075 0.00018 0.00000 0.00738 0.00738 -3.13505

D174 0.02019 -0.00002 0.00000 -0.00072 -0.00073 0.01946

D175 0.00056 0.00017 0.00000 0.00700 0.00700 0.00755

D176 -3.12001 -0.00003 0.00000 -0.00111 -0.00111 -3.12113

D177 0.01796 -0.00029 0.00000 -0.01208 -0.01209 0.00587

D178 -3.12384 -0.00012 0.00000 -0.00537 -0.00539 -3.12923

D179 3.13800 -0.00015 0.00000 -0.00619 -0.00619 3.13180

D180 -0.00381 0.00002 0.00000 0.00051 0.00051 -0.00330

D181 -0.00647 0.00016 0.00000 0.00616 0.00613 -0.00034

D182 3.13327 0.00016 0.00000 0.00629 0.00626 3.13953

D183 3.13533 -0.00000 0.00000 -0.00057 -0.00059 3.13474

D184 -0.00811 -0.00000 0.00000 -0.00045 -0.00046 -0.00857

D185 -0.00783 0.00016 0.00000 0.00642 0.00638 -0.00144

D186 3.13169 -0.00000 0.00000 -0.00012 -0.00013 3.13156

D187 3.13561 0.00016 0.00000 0.00629 0.00626 -3.14131

D188 -0.00805 -0.00000 0.00000 -0.00024 -0.00026 -0.00831

D189 0.01077 -0.00032 0.00000 -0.01301 -0.01303 -0.00227

D190 3.13123 -0.00012 0.00000 -0.00490 -0.00490 3.12633

D191 -3.12876 -0.00016 0.00000 -0.00651 -0.00654 -3.13530

D192 -0.00830 0.00004 0.00000 0.00161 0.00160 -0.00670

D193 -3.12808 -0.00013 0.00000 -0.00516 -0.00516 -3.13324

D194 -0.00793 0.00001 0.00000 0.00071 0.00072 -0.00721

D195 0.01490 -0.00014 0.00000 -0.00555 -0.00555 0.00935

D196 3.13505 0.00000 0.00000 0.00033 0.00033 3.13538

D197 -3.14075 -0.00018 0.00000 -0.00738 -0.00738 3.13505

D198 -0.02019 0.00002 0.00000 0.00072 0.00073 -0.01946

D199 -0.00056 -0.00017 0.00000 -0.00700 -0.00700 -0.00755

D200 3.12001 0.00003 0.00000 0.00111 0.00111 3.12113

D201 -0.01796 0.00029 0.00000 0.01208 0.01209 -0.00587

D202 3.12384 0.00012 0.00000 0.00537 0.00539 3.12923

D203 -3.13800 0.00015 0.00000 0.00619 0.00619 -3.13180

D204 0.00381 -0.00002 0.00000 -0.00051 -0.00051 0.00330

D205 0.00647 -0.00016 0.00000 -0.00616 -0.00613 0.00034

D206 -3.13327 -0.00016 0.00000 -0.00629 -0.00626 -3.13953

D207 -3.13533 0.00000 0.00000 0.00057 0.00059 -3.13474

D208 0.00811 0.00000 0.00000 0.00045 0.00046 0.00857

D209 0.00783 -0.00016 0.00000 -0.00642 -0.00638 0.00144

D210 -3.13169 0.00000 0.00000 0.00012 0.00013 -3.13156

D211 -3.13561 -0.00016 0.00000 -0.00629 -0.00626 3.14131

D212 0.00805 0.00000 0.00000 0.00024 0.00026 0.00831

D213 -0.01077 0.00032 0.00000 0.01301 0.01303 0.00227

D214 -3.13123 0.00012 0.00000 0.00490 0.00490 -3.12633

D215 3.12876 0.00016 0.00000 0.00651 0.00654 3.13530

D216 0.00830 -0.00004 0.00000 -0.00161 -0.00160 0.00670

Item Value Threshold Converged?

Maximum Force 0.006821 0.000450 NO

RMS Force 0.001298 0.000300 NO

Maximum Displacement 0.216908 0.001800 NO

RMS Displacement 0.057633 0.001200 NO

Predicted change in Energy=-1.611883D-03

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Aug 18 13:52:28 2019, MaxMem= 2013265920 cpu: 1.7

(Enter /home/kira/g09/l202.exe)

Stoichiometry C44H30N4(1-,2)

Framework group CS[SG(H2N2),X(C44H28N2)]

Deg. of freedom 116

Full point group CS NOp 2

RotChk: IX=3 Diff= 2.00D+00

Largest Abelian subgroup CS NOp 2

Largest concise Abelian subgroup CS NOp 2

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 4.234709 -0.344829 0.682758

2 6 0 2.894278 -0.087706 1.142211

3 7 0 2.120883 0.028483 0.000000

4 6 0 2.894278 -0.087706 -1.142211

5 6 0 4.234709 -0.344829 -0.682758

6 6 0 2.461814 0.026210 -2.458374

7 6 0 1.097410 0.179416 -2.867291

8 7 0 0.000248 0.012949 -2.058472

9 6 0 -1.096327 0.184031 -2.867133

10 6 0 -0.687789 0.516058 -4.202706

11 6 0 0.690053 0.512625 -4.203016

12 6 0 2.461814 0.026210 2.458374

13 6 0 1.097410 0.179416 2.867291

14 6 0 0.690053 0.512625 4.203016

15 6 0 -0.687789 0.516058 4.202706

16 6 0 -1.096327 0.184031 2.867133

17 7 0 0.000248 0.012949 2.058472

18 6 0 -2.461465 0.034386 2.458694

19 6 0 -2.894507 -0.075654 1.142243

20 6 0 -4.232743 -0.343483 0.682780

21 6 0 -4.232743 -0.343483 -0.682780

22 6 0 -2.894507 -0.075654 -1.142243

23 7 0 -2.122357 0.046632 -0.000000

24 6 0 -2.461465 0.034386 -2.458694

25 6 0 3.501244 -0.010065 -3.525171

26 6 0 4.548582 0.922535 -3.552642

27 6 0 5.520630 0.880049 -4.550762

28 6 0 5.463729 -0.095369 -5.544403

29 6 0 4.425641 -1.027218 -5.532879

30 6 0 3.454250 -0.982191 -4.536461

31 6 0 5.463729 -0.095369 5.544403

32 6 0 5.520630 0.880049 4.550762

33 6 0 4.548582 0.922535 3.552642

34 6 0 3.501244 -0.010065 3.525171

35 6 0 3.454250 -0.982191 4.536461

36 6 0 4.425641 -1.027218 5.532879

37 6 0 -3.500533 -0.006393 -3.525170

38 6 0 -3.448033 -0.976853 -4.538022

39 6 0 -4.420715 -1.027949 -5.532788

40 6 0 -5.465865 -0.103955 -5.541430

41 6 0 -5.528386 0.869753 -4.546462

42 6 0 -4.555021 0.918372 -3.549933

43 6 0 -3.500533 -0.006393 3.525170

44 6 0 -3.448033 -0.976853 4.538022

45 6 0 -4.420715 -1.027949 5.532788

46 6 0 -5.465865 -0.103955 5.541430

47 6 0 -5.528386 0.869753 4.546462

48 6 0 -4.555021 0.918372 3.549933

49 1 0 5.079529 -0.524892 1.328330

50 1 0 5.079529 -0.524892 -1.328330

51 1 0 -1.341480 0.737670 -5.033533

52 1 0 1.344364 0.731054 -5.034179

53 1 0 1.344364 0.731054 5.034179

54 1 0 -1.341480 0.737670 5.033533

55 1 0 -5.075477 -0.532714 1.328464

56 1 0 -5.075477 -0.532714 -1.328464

57 1 0 4.590892 1.692827 -2.790917

58 1 0 6.318947 1.615334 -4.556059

59 1 0 6.219905 -0.128877 -6.321986

60 1 0 4.376196 -1.794471 -6.298978

61 1 0 2.655068 -1.714414 -4.528724

62 1 0 6.219905 -0.128877 6.321986

63 1 0 6.318947 1.615334 4.556059

64 1 0 4.590892 1.692827 2.790917

65 1 0 2.655068 -1.714414 4.528724

66 1 0 4.376196 -1.794471 6.298978

67 1 0 -2.643885 -1.703577 -4.532256

68 1 0 -4.366903 -1.794026 -6.299769

69 1 0 -6.223139 -0.142271 -6.317719

70 1 0 -6.332205 1.599029 -4.549524

71 1 0 -4.602016 1.687361 -2.787180

72 1 0 -2.643885 -1.703577 4.532256

73 1 0 -4.366903 -1.794026 6.299769

74 1 0 -6.223139 -0.142271 6.317719

75 1 0 -6.332205 1.599029 4.549524

76 1 0 -4.602016 1.687361 2.787180

77 1 0 1.115626 0.127416 0.000000

78 1 0 -1.119828 0.168193 -0.000000

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

Rotational constants (GHZ): 0.0586376 0.0578465 0.0299661

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(Enter /home/kira/g09/l301.exe)

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

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

There are 513 symmetry adapted cartesian basis functions of A' symmetry.

There are 489 symmetry adapted cartesian basis functions of A" symmetry.

There are 488 symmetry adapted basis functions of A' symmetry.

There are 466 symmetry adapted basis functions of A" symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 161 beta electrons

nuclear repulsion energy 5348.1959463494 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= 78 NActive= 78 NUniq= 41 SFac= 3.62D+00 NAtFMM= 60 NAOKFM=T 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= -0.2119577815 Hartrees.

Nuclear repulsion after empirical dispersion term = 5347.9839885679 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= 78.

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

Smoothing algorithm: York/Karplus (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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5780

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.96D-09

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 212

GePol: Fraction of low-weight points (<1% of avg) = 3.67%

GePol: Cavity surface area = 613.281 Ang\*\*2

GePol: Cavity volume = 627.776 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0020803598 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5347.9819082081 Hartrees.

Leave Link 301 at Sun Aug 18 13:52:28 2019, MaxMem= 2013265920 cpu: 1.0

(Enter /home/kira/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.

One-electron integral symmetry used in STVInt

NBasis= 954 RedAO= T EigKep= 9.27D-05 NBF= 488 466

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 488 466

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= 940 940 940 940 940 MxSgAt= 78 MxSgA2= 78.

Leave Link 302 at Sun Aug 18 13:52:29 2019, MaxMem= 2013265920 cpu: 10.3

(Enter /home/kira/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sun Aug 18 13:52:29 2019, MaxMem= 2013265920 cpu: 1.3

(Enter /home/kira/g09/l401.exe)

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

B after Tr= 0.000000 -0.000000 0.000000

Rot= 0.707114 -0.000000 -0.000000 -0.707099 Ang= -90.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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The electronic state of the initial guess is 2-A'.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7586 S= 0.5043

Generating alternative initial guess.

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2000

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= -1914.57667632200

Leave Link 401 at Sun Aug 18 13:52:36 2019, MaxMem= 2013265920 cpu: 49.8

(Enter /home/kira/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3047318 IEndB= 3047318 NGot= 2013265920 MDV= 2011240249

LenX= 2011240249 LenY= 2010235243

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= 480000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 100225200.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.88D-15 for 5758.

Iteration 1 A\*A^-1 deviation from orthogonality is 5.09D-15 for 4718 2507.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.44D-15 for 5769.

Iteration 1 A^-1\*A deviation from orthogonality is 3.04D-14 for 4870 4836.

E= -1914.46698619741

DIIS: error= 4.37D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.46698619741 IErMin= 1 ErrMin= 4.37D-03

ErrMax= 4.37D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.85D-02 BMatP= 4.85D-02

IDIUse=3 WtCom= 9.56D-01 WtEn= 4.37D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.446 Goal= None Shift= 0.000

Gap= 0.502 Goal= None Shift= 0.000

GapD= 0.446 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=1.69D-04 MaxDP=5.98D-03 OVMax= 2.43D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.69D-04 CP: 9.99D-01

E= -1914.49198349901 Delta-E= -0.024997301592 Rises=F Damp=F

DIIS: error= 5.36D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.49198349901 IErMin= 2 ErrMin= 5.36D-04

ErrMax= 5.36D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.00D-03 BMatP= 4.85D-02

IDIUse=3 WtCom= 9.95D-01 WtEn= 5.36D-03

Coeff-Com: -0.539D-01 0.105D+01

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

Coeff: -0.536D-01 0.105D+01

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=3.55D-05 MaxDP=1.94D-03 DE=-2.50D-02 OVMax= 5.99D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.31D-05 CP: 1.00D+00 1.08D+00

E= -1914.49225202617 Delta-E= -0.000268527167 Rises=F Damp=F

DIIS: error= 5.39D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.49225202617 IErMin= 2 ErrMin= 5.36D-04

ErrMax= 5.39D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.01D-03 BMatP= 1.00D-03

IDIUse=3 WtCom= 9.95D-01 WtEn= 5.39D-03

Coeff-Com: -0.418D-01 0.557D+00 0.485D+00

Coeff-En: 0.000D+00 0.475D-01 0.953D+00

Coeff: -0.416D-01 0.554D+00 0.488D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=1.70D-05 MaxDP=1.55D-03 DE=-2.69D-04 OVMax= 3.67D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.27D-05 CP: 9.99D-01 1.09D+00 6.61D-01

E= -1914.49245803804 Delta-E= -0.000206011864 Rises=F Damp=F

DIIS: error= 1.80D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.49245803804 IErMin= 4 ErrMin= 1.80D-04

ErrMax= 1.80D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.63D-05 BMatP= 1.00D-03

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.80D-03

Coeff-Com: -0.120D-01 0.125D+00 0.256D+00 0.631D+00

Coeff-En: 0.000D+00 0.000D+00 0.480D-01 0.952D+00

Coeff: -0.120D-01 0.125D+00 0.255D+00 0.632D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=6.07D-06 MaxDP=3.99D-04 DE=-2.06D-04 OVMax= 1.41D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.22D-06 CP: 9.99D-01 1.09D+00 7.24D-01 7.08D-01

E= -1914.49247889847 Delta-E= -0.000020860432 Rises=F Damp=F

DIIS: error= 5.91D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.49247889847 IErMin= 5 ErrMin= 5.91D-05

ErrMax= 5.91D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.23D-06 BMatP= 9.63D-05

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

Coeff-Com: -0.288D-02 0.184D-01 0.897D-01 0.322D+00 0.573D+00

Coeff: -0.288D-02 0.184D-01 0.897D-01 0.322D+00 0.573D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=2.38D-06 MaxDP=1.54D-04 DE=-2.09D-05 OVMax= 4.83D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.72D-06 CP: 9.99D-01 1.09D+00 7.23D-01 7.87D-01 6.94D-01

E= -1914.49248088707 Delta-E= -0.000001988603 Rises=F Damp=F

DIIS: error= 2.02D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.49248088707 IErMin= 6 ErrMin= 2.02D-05

ErrMax= 2.02D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.69D-06 BMatP= 9.23D-06

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

Coeff-Com: 0.692D-03-0.151D-01-0.382D-03 0.571D-01 0.331D+00 0.627D+00

Coeff: 0.692D-03-0.151D-01-0.382D-03 0.571D-01 0.331D+00 0.627D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=9.15D-07 MaxDP=4.98D-05 DE=-1.99D-06 OVMax= 1.87D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 3.64D-07 CP: 9.99D-01 1.09D+00 7.35D-01 7.89D-01 7.75D-01

CP: 6.18D-01

E= -1914.49248131784 Delta-E= -0.000000430767 Rises=F Damp=F

DIIS: error= 5.48D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.49248131784 IErMin= 7 ErrMin= 5.48D-06

ErrMax= 5.48D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.90D-08 BMatP= 1.69D-06

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

Coeff-Com: 0.441D-03-0.829D-02-0.300D-02 0.192D-01 0.152D+00 0.326D+00

Coeff-Com: 0.514D+00

Coeff: 0.441D-03-0.829D-02-0.300D-02 0.192D-01 0.152D+00 0.326D+00

Coeff: 0.514D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=2.06D-07 MaxDP=1.17D-05 DE=-4.31D-07 OVMax= 4.78D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.67D-07 CP: 9.99D-01 1.09D+00 7.34D-01 7.91D-01 7.75D-01

CP: 6.73D-01 8.27D-01

E= -1914.49248133972 Delta-E= -0.000000021883 Rises=F Damp=F

DIIS: error= 2.11D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.49248133972 IErMin= 8 ErrMin= 2.11D-06

ErrMax= 2.11D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.22D-08 BMatP= 7.90D-08

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

Coeff-Com: 0.481D-04-0.402D-03-0.142D-02-0.420D-02-0.457D-02 0.139D-01

Coeff-Com: 0.238D+00 0.759D+00

Coeff: 0.481D-04-0.402D-03-0.142D-02-0.420D-02-0.457D-02 0.139D-01

Coeff: 0.238D+00 0.759D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=1.06D-07 MaxDP=7.60D-06 DE=-2.19D-08 OVMax= 3.14D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 7.61D-08 CP: 9.99D-01 1.09D+00 7.34D-01 7.90D-01 7.79D-01

CP: 6.70D-01 1.01D+00 1.04D+00

E= -1914.49248134679 Delta-E= -0.000000007064 Rises=F Damp=F

DIIS: error= 2.06D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.49248134679 IErMin= 9 ErrMin= 2.06D-06

ErrMax= 2.06D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.27D-09 BMatP= 1.22D-08

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

Coeff-Com: -0.106D-03 0.229D-02 0.203D-03-0.790D-02-0.489D-01-0.900D-01

Coeff-Com: -0.243D-01 0.410D+00 0.759D+00

Coeff: -0.106D-03 0.229D-02 0.203D-03-0.790D-02-0.489D-01-0.900D-01

Coeff: -0.243D-01 0.410D+00 0.759D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=7.83D-08 MaxDP=4.87D-06 DE=-7.06D-09 OVMax= 2.51D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 4.68D-08 CP: 9.99D-01 1.09D+00 7.34D-01 7.91D-01 7.81D-01

CP: 6.83D-01 1.10D+00 1.32D+00 1.06D+00

E= -1914.49248135019 Delta-E= -0.000000003406 Rises=F Damp=F

DIIS: error= 1.51D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.49248135019 IErMin=10 ErrMin= 1.51D-06

ErrMax= 1.51D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.33D-09 BMatP= 4.27D-09

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

Coeff-Com: -0.676D-04 0.125D-02 0.608D-03-0.241D-02-0.227D-01-0.489D-01

Coeff-Com: -0.950D-01-0.590D-01 0.396D+00 0.830D+00

Coeff: -0.676D-04 0.125D-02 0.608D-03-0.241D-02-0.227D-01-0.489D-01

Coeff: -0.950D-01-0.590D-01 0.396D+00 0.830D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=5.08D-08 MaxDP=2.55D-06 DE=-3.41D-09 OVMax= 1.59D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 2.38D-08 CP: 9.99D-01 1.09D+00 7.34D-01 7.91D-01 7.81D-01

CP: 6.86D-01 1.18D+00 1.40D+00 1.47D+00 1.19D+00

E= -1914.49248135143 Delta-E= -0.000000001240 Rises=F Damp=F

DIIS: error= 7.68D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.49248135143 IErMin=11 ErrMin= 7.68D-07

ErrMax= 7.68D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.31D-10 BMatP= 1.33D-09

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

Coeff-Com: 0.395D-05-0.210D-03 0.260D-03 0.168D-02 0.622D-02 0.799D-02

Coeff-Com: -0.384D-01-0.168D+00-0.732D-01 0.419D+00 0.845D+00

Coeff: 0.395D-05-0.210D-03 0.260D-03 0.168D-02 0.622D-02 0.799D-02

Coeff: -0.384D-01-0.168D+00-0.732D-01 0.419D+00 0.845D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=2.74D-08 MaxDP=1.23D-06 DE=-1.24D-09 OVMax= 8.84D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.08D-08 CP: 9.99D-01 1.09D+00 7.34D-01 7.91D-01 7.81D-01

CP: 6.87D-01 1.20D+00 1.48D+00 1.64D+00 1.50D+00

CP: 1.13D+00

E= -1914.49248135185 Delta-E= -0.000000000417 Rises=F Damp=F

DIIS: error= 2.50D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.49248135185 IErMin=12 ErrMin= 2.50D-07

ErrMax= 2.50D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.24D-11 BMatP= 3.31D-10

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

Coeff-Com: 0.111D-04-0.250D-03-0.129D-04 0.902D-03 0.536D-02 0.990D-02

Coeff-Com: 0.275D-02-0.428D-01-0.834D-01 0.177D-01 0.249D+00 0.841D+00

Coeff: 0.111D-04-0.250D-03-0.129D-04 0.902D-03 0.536D-02 0.990D-02

Coeff: 0.275D-02-0.428D-01-0.834D-01 0.177D-01 0.249D+00 0.841D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=8.70D-09 MaxDP=4.31D-07 DE=-4.17D-10 OVMax= 2.93D-06

Error on total polarization charges = 0.08639

SCF Done: E(UB3LYP) = -1914.49248135 A.U. after 12 cycles

NFock= 12 Conv=0.87D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7586 S= 0.5043

<L.S>= 0.000000000000E+00

KE= 1.906518725626D+03 PE=-1.518072514078D+04 EE= 6.011732025598D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.31

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7586, after 0.7500

Leave Link 502 at Sun Aug 18 13:59:53 2019, MaxMem= 2013265920 cpu: 3481.6

(Enter /home/kira/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 = 186

Leave Link 701 at Sun Aug 18 14:00:10 2019, MaxMem= 2013265920 cpu: 138.8

(Enter /home/kira/g09/l702.exe)

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

Leave Link 702 at Sun Aug 18 14:00:10 2019, MaxMem= 2013265920 cpu: 0.1

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 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= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

Petite list used in FoFCou.

Leave Link 703 at Sun Aug 18 14:01:25 2019, MaxMem= 2013265920 cpu: 600.2

(Enter /home/kira/g09/l716.exe)

Dipole =-3.09356047D-03-1.36834978D-01 1.52766688D-13

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.001441417 -0.000053092 -0.002851389

2 6 -0.001135112 -0.000570558 0.002646643

3 7 -0.001470697 0.000572243 -0.000000000

4 6 -0.001135112 -0.000570558 -0.002646643

5 6 0.001441417 -0.000053092 0.002851389

6 6 -0.000072585 0.000140228 0.002198495

7 6 -0.000990701 0.000400640 0.000856751

8 7 -0.000005870 -0.000437020 0.000221087

9 6 0.000909941 0.000461727 0.000866726

10 6 0.001137203 -0.000158097 -0.000886165

11 6 -0.001125737 -0.000071577 -0.000840420

12 6 -0.000072585 0.000140228 -0.002198495

13 6 -0.000990701 0.000400640 -0.000856751

14 6 -0.001125737 -0.000071577 0.000840419

15 6 0.001137203 -0.000158097 0.000886165

16 6 0.000909941 0.000461727 -0.000866726

17 7 -0.000005870 -0.000437020 -0.000221087

18 6 0.000144531 0.000247713 -0.002236672

19 6 0.001186661 -0.000780625 0.002626503

20 6 -0.001494925 -0.000005560 -0.002877334

21 6 -0.001494925 -0.000005560 0.002877334

22 6 0.001186662 -0.000780625 -0.002626503

23 7 0.001393088 0.000757244 0.000000000

24 6 0.000144531 0.000247713 0.002236672

25 6 0.000575037 -0.000102787 -0.000782189

26 6 -0.000413828 -0.000281134 -0.000242722

27 6 -0.000140731 0.000203996 0.000168229

28 6 -0.000043816 -0.000018470 -0.000008254

29 6 -0.000169607 -0.000151596 0.000156832

30 6 0.000243827 0.000302080 0.000440979

31 6 -0.000043816 -0.000018470 0.000008254

32 6 -0.000140731 0.000203996 -0.000168229

33 6 -0.000413828 -0.000281134 0.000242721

34 6 0.000575037 -0.000102787 0.000782189

35 6 0.000243827 0.000302080 -0.000440979

36 6 -0.000169607 -0.000151596 -0.000156832

37 6 -0.000624183 -0.000143383 -0.000827875

38 6 -0.000257335 0.000304581 0.000467666

39 6 0.000160045 -0.000146484 0.000148993

40 6 0.000049950 -0.000016529 -0.000011063

41 6 0.000145147 0.000213681 0.000164874

42 6 0.000432784 -0.000262208 -0.000260691

43 6 -0.000624183 -0.000143383 0.000827875

44 6 -0.000257335 0.000304581 -0.000467666

45 6 0.000160045 -0.000146484 -0.000148993

46 6 0.000049950 -0.000016529 0.000011063

47 6 0.000145147 0.000213681 -0.000164874

48 6 0.000432784 -0.000262208 0.000260691

49 1 0.000159635 0.000202724 0.000039753

50 1 0.000159635 0.000202724 -0.000039753

51 1 -0.000009060 -0.000135154 -0.000103913

52 1 0.000024963 -0.000126947 -0.000100660

53 1 0.000024963 -0.000126947 0.000100660

54 1 -0.000009060 -0.000135154 0.000103913

55 1 -0.000160062 0.000188861 0.000018867

56 1 -0.000160062 0.000188861 -0.000018867

57 1 0.000111621 0.000200548 0.000155506

58 1 -0.000042638 -0.000003001 0.000168609

59 1 -0.000044304 -0.000002460 0.000055959

60 1 -0.000172740 0.000016543 0.000053682

61 1 -0.000209425 -0.000210091 -0.000109959

62 1 -0.000044304 -0.000002460 -0.000055959

63 1 -0.000042638 -0.000003001 -0.000168609

64 1 0.000111621 0.000200548 -0.000155506

65 1 -0.000209425 -0.000210091 0.000109959

66 1 -0.000172740 0.000016543 -0.000053682

67 1 0.000217533 -0.000205553 -0.000112937

68 1 0.000174397 0.000019653 0.000052174

69 1 0.000045104 -0.000001009 0.000056998

70 1 0.000041523 -0.000002979 0.000172703

71 1 -0.000112590 0.000201636 0.000147249

72 1 0.000217533 -0.000205553 0.000112937

73 1 0.000174397 0.000019653 -0.000052174

74 1 0.000045104 -0.000001009 -0.000056998

75 1 0.000041523 -0.000002979 -0.000172703

76 1 -0.000112590 0.000201636 -0.000147249

77 1 -0.000475175 0.000192286 -0.000000000

78 1 0.000600641 0.000041629 0.000000000

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

Cartesian Forces: Max 0.002877334 RMS 0.000736278

Leave Link 716 at Sun Aug 18 14:01:25 2019, MaxMem= 2013265920 cpu: 0.2

(Enter /home/kira/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 0.002335190 RMS 0.000446300

Search for a local minimum.

Step number 2 out of a maximum of 452

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

RMS Force = .44630D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 1 2

DE= -1.69D-03 DEPred=-1.61D-03 R= 1.05D+00

TightC=F SS= 1.41D+00 RLast= 2.31D-01 DXNew= 5.0454D-01 6.9190D-01

Trust test= 1.05D+00 RLast= 2.31D-01 DXMaxT set to 5.05D-01

ITU= 1 0

Use linear search instead of GDIIS.

Eigenvalues --- 0.00963 0.00983 0.00985 0.00988 0.01533

Eigenvalues --- 0.01613 0.01614 0.01619 0.01650 0.01663

Eigenvalues --- 0.01721 0.01721 0.01721 0.01721 0.01738

Eigenvalues --- 0.01751 0.01777 0.01789 0.01795 0.01801

Eigenvalues --- 0.01834 0.01836 0.01855 0.01860 0.01892

Eigenvalues --- 0.01904 0.01932 0.01942 0.01945 0.01982

Eigenvalues --- 0.01993 0.02012 0.02022 0.02028 0.02043

Eigenvalues --- 0.02052 0.02068 0.02069 0.02070 0.02070

Eigenvalues --- 0.02084 0.02108 0.02118 0.02119 0.02119

Eigenvalues --- 0.02119 0.02130 0.02132 0.02132 0.02133

Eigenvalues --- 0.02133 0.02133 0.02135 0.02160 0.02160

Eigenvalues --- 0.02160 0.02161 0.02162 0.02162 0.02162

Eigenvalues --- 0.02173 0.02173 0.02173 0.02173 0.02181

Eigenvalues --- 0.02181 0.02181 0.02182 0.02186 0.02186

Eigenvalues --- 0.02187 0.02187 0.02216 0.02217 0.02219

Eigenvalues --- 0.15956 0.15977 0.15991 0.15993 0.15995

Eigenvalues --- 0.15996 0.15996 0.15996 0.15998 0.15998

Eigenvalues --- 0.15998 0.15998 0.15998 0.15998 0.15999

Eigenvalues --- 0.15999 0.15999 0.15999 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16044

Eigenvalues --- 0.22000 0.22000 0.22000 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22005 0.22743 0.22763

Eigenvalues --- 0.22800 0.22818 0.23420 0.23469 0.23469

Eigenvalues --- 0.23469 0.23533 0.23821 0.24121 0.24592

Eigenvalues --- 0.24665 0.24745 0.24930 0.24943 0.24997

Eigenvalues --- 0.24998 0.24999 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.28167 0.33981 0.34159 0.34182

Eigenvalues --- 0.34206 0.35405 0.35413 0.35413 0.35413

Eigenvalues --- 0.35414 0.35415 0.35416 0.35416 0.35416

Eigenvalues --- 0.35416 0.35416 0.35417 0.35506 0.35507

Eigenvalues --- 0.35508 0.35521 0.35542 0.35544 0.35547

Eigenvalues --- 0.35635 0.36039 0.36056 0.36057 0.36058

Eigenvalues --- 0.36239 0.36250 0.36250 0.36251 0.37114

Eigenvalues --- 0.37154 0.37262 0.37295 0.38108 0.39122

Eigenvalues --- 0.39731 0.39797 0.40229 0.40356 0.40422

Eigenvalues --- 0.40446 0.41302 0.41795 0.41803 0.41810

Eigenvalues --- 0.42081 0.42081 0.42085 0.42085 0.42240

Eigenvalues --- 0.43232 0.44642 0.45029 0.45382 0.45571

Eigenvalues --- 0.45572 0.45588 0.45588 0.45666 0.45770

Eigenvalues --- 0.45850 0.45930 0.45935 0.45940 0.45942

Eigenvalues --- 0.45958 0.45962 0.46660 0.46661 0.46661

Eigenvalues --- 0.46668 0.47073 0.47079 0.47086 0.47415

Eigenvalues --- 0.48174 0.48275 0.49325 0.49425 0.49964

Eigenvalues --- 0.50528 0.50799 0.54271

RFO step: Lambda=-6.96967825D-04 EMin= 9.62532209D-03

Quartic linear search produced a step of 0.13299.

Iteration 1 RMS(Cart)= 0.05487561 RMS(Int)= 0.00062689

Iteration 2 RMS(Cart)= 0.00125105 RMS(Int)= 0.00006926

Iteration 3 RMS(Cart)= 0.00000060 RMS(Int)= 0.00006926

ITry= 1 IFail=0 DXMaxC= 2.50D-01 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.73D-08 for atom 50.

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

(Linear) (Quad) (Total)

R1 2.72145 0.00163 0.00101 0.00484 0.00589 2.72733

R2 2.58045 -0.00230 -0.00024 -0.00588 -0.00603 2.57443

R3 2.03784 0.00011 0.00012 0.00043 0.00055 2.03840

R4 2.61595 0.00046 0.00148 0.00252 0.00392 2.61987

R5 2.62685 -0.00231 -0.00196 -0.00679 -0.00875 2.61810

R6 2.61595 0.00046 0.00148 0.00252 0.00392 2.61987

R7 1.90884 0.00049 -0.00030 0.00104 0.00074 1.90958

R8 2.72145 0.00163 0.00101 0.00484 0.00589 2.72733

R9 2.62685 -0.00231 -0.00196 -0.00679 -0.00875 2.61810

R10 2.03784 0.00011 0.00012 0.00043 0.00055 2.03840

R11 2.70718 -0.00086 -0.00024 -0.00252 -0.00276 2.70442

R12 2.81549 -0.00025 0.00158 0.00007 0.00165 2.81714

R13 2.59496 -0.00100 0.00060 -0.00161 -0.00110 2.59386

R14 2.71301 0.00068 0.00071 0.00216 0.00291 2.71592

R15 2.59497 -0.00101 0.00061 -0.00161 -0.00108 2.59390

R16 2.71286 0.00072 0.00071 0.00230 0.00304 2.71590

R17 2.70754 -0.00090 -0.00026 -0.00265 -0.00290 2.70463

R18 2.60375 -0.00161 0.00020 -0.00388 -0.00358 2.60017

R19 2.04117 0.00006 0.00016 0.00027 0.00044 2.04160

R20 2.04114 0.00007 0.00016 0.00030 0.00046 2.04160

R21 2.70718 -0.00086 -0.00024 -0.00252 -0.00276 2.70442

R22 2.81549 -0.00025 0.00158 0.00007 0.00165 2.81714

R23 2.71301 0.00068 0.00071 0.00216 0.00291 2.71592

R24 2.59496 -0.00100 0.00060 -0.00161 -0.00110 2.59386

R25 2.60375 -0.00161 0.00020 -0.00388 -0.00358 2.60017

R26 2.04114 0.00007 0.00016 0.00030 0.00046 2.04160

R27 2.71286 0.00072 0.00071 0.00230 0.00304 2.71590

R28 2.04117 0.00006 0.00016 0.00027 0.00044 2.04160

R29 2.59497 -0.00101 0.00061 -0.00161 -0.00108 2.59390

R30 2.70754 -0.00090 -0.00026 -0.00265 -0.00290 2.70463

R31 2.62711 -0.00226 -0.00195 -0.00664 -0.00860 2.61851

R32 2.81480 -0.00019 0.00159 0.00029 0.00188 2.81669

R33 2.72128 0.00167 0.00101 0.00496 0.00601 2.72729

R34 2.61568 0.00049 0.00147 0.00260 0.00399 2.61967

R35 2.58054 -0.00234 -0.00024 -0.00597 -0.00611 2.57443

R36 2.03785 0.00010 0.00012 0.00039 0.00052 2.03837

R37 2.72128 0.00167 0.00101 0.00496 0.00601 2.72729

R38 2.03785 0.00010 0.00012 0.00039 0.00052 2.03837

R39 2.61568 0.00049 0.00147 0.00260 0.00399 2.61967

R40 2.62711 -0.00226 -0.00195 -0.00664 -0.00860 2.61851

R41 1.90838 0.00060 -0.00030 0.00131 0.00101 1.90939

R42 2.81480 -0.00019 0.00159 0.00029 0.00188 2.81669

R43 2.65061 -0.00051 0.00009 -0.00128 -0.00119 2.64942

R44 2.65232 -0.00055 0.00014 -0.00137 -0.00123 2.65109

R45 2.63407 -0.00042 0.00041 -0.00076 -0.00036 2.63371

R46 2.04873 0.00026 0.00002 0.00082 0.00084 2.04957

R47 2.63344 0.00019 -0.00007 0.00048 0.00041 2.63385

R48 2.05101 -0.00003 0.00013 -0.00004 0.00009 2.05110

R49 2.63622 0.00015 -0.00006 0.00039 0.00033 2.63655

R50 2.05064 -0.00007 0.00008 -0.00018 -0.00010 2.05054

R51 2.63105 -0.00044 0.00039 -0.00083 -0.00044 2.63061

R52 2.05105 -0.00004 0.00013 -0.00006 0.00007 2.05112

R53 2.04833 0.00030 0.00004 0.00096 0.00099 2.04932

R54 2.63344 0.00019 -0.00007 0.00048 0.00041 2.63385

R55 2.63622 0.00015 -0.00006 0.00039 0.00033 2.63655

R56 2.05064 -0.00007 0.00008 -0.00018 -0.00010 2.05054

R57 2.63407 -0.00042 0.00041 -0.00076 -0.00036 2.63371

R58 2.05101 -0.00003 0.00013 -0.00004 0.00009 2.05110

R59 2.65061 -0.00051 0.00009 -0.00128 -0.00119 2.64942

R60 2.04873 0.00026 0.00002 0.00082 0.00084 2.04957

R61 2.65232 -0.00055 0.00014 -0.00137 -0.00123 2.65109

R62 2.63105 -0.00044 0.00039 -0.00083 -0.00044 2.63061

R63 2.04833 0.00030 0.00004 0.00096 0.00099 2.04932

R64 2.05105 -0.00004 0.00013 -0.00006 0.00007 2.05112

R65 2.65264 -0.00057 0.00013 -0.00141 -0.00128 2.65136

R66 2.65084 -0.00051 0.00009 -0.00129 -0.00121 2.64964

R67 2.63092 -0.00043 0.00040 -0.00080 -0.00041 2.63051

R68 2.04825 0.00030 0.00004 0.00097 0.00101 2.04926

R69 2.63627 0.00014 -0.00006 0.00038 0.00032 2.63659

R70 2.05105 -0.00004 0.00013 -0.00006 0.00007 2.05112

R71 2.63342 0.00018 -0.00007 0.00047 0.00040 2.63383

R72 2.05064 -0.00007 0.00008 -0.00018 -0.00011 2.05054

R73 2.63403 -0.00042 0.00041 -0.00077 -0.00036 2.63367

R74 2.05101 -0.00003 0.00013 -0.00003 0.00009 2.05110

R75 2.04871 0.00025 0.00002 0.00081 0.00082 2.04954

R76 2.65264 -0.00057 0.00013 -0.00141 -0.00128 2.65136

R77 2.65084 -0.00051 0.00009 -0.00129 -0.00121 2.64964

R78 2.63092 -0.00043 0.00040 -0.00080 -0.00041 2.63051

R79 2.04825 0.00030 0.00004 0.00097 0.00101 2.04926

R80 2.63627 0.00014 -0.00006 0.00038 0.00032 2.63659

R81 2.05105 -0.00004 0.00013 -0.00006 0.00007 2.05112

R82 2.63342 0.00018 -0.00007 0.00047 0.00040 2.63383

R83 2.05064 -0.00007 0.00008 -0.00018 -0.00011 2.05054

R84 2.63403 -0.00042 0.00041 -0.00077 -0.00036 2.63367

R85 2.05101 -0.00003 0.00013 -0.00003 0.00009 2.05110

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A3 2.21261 -0.00010 -0.00034 -0.00047 -0.00078 2.21183

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A7 1.94082 -0.00097 0.00132 -0.00323 -0.00194 1.93888

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D125 -3.13563 -0.00003 -0.00068 -0.00232 -0.00300 -3.13863

D126 -0.00866 0.00001 0.00009 0.00051 0.00061 -0.00805

D127 0.00917 -0.00000 -0.00075 -0.00045 -0.00120 0.00797

D128 3.13614 0.00004 0.00003 0.00238 0.00241 3.13856

D129 0.00217 0.00001 0.00171 0.00167 0.00338 0.00555

D130 3.13526 0.00004 0.00086 0.00267 0.00353 3.13879

D131 -3.12622 -0.00001 0.00064 -0.00021 0.00044 -3.12578

D132 0.00687 0.00002 -0.00021 0.00079 0.00059 0.00746

D133 0.00144 -0.00001 -0.00084 -0.00067 -0.00151 -0.00007

D134 3.14121 -0.00000 -0.00082 -0.00066 -0.00147 3.13974

D135 -3.13163 -0.00003 0.00002 -0.00167 -0.00165 -3.13328

D136 0.00815 -0.00003 0.00004 -0.00165 -0.00161 0.00654

D137 0.00035 -0.00001 -0.00081 -0.00086 -0.00166 -0.00131

D138 -3.13501 -0.00004 0.00008 -0.00217 -0.00208 -3.13709

D139 -3.13942 -0.00001 -0.00083 -0.00088 -0.00170 -3.14113

D140 0.00840 -0.00004 0.00006 -0.00218 -0.00212 0.00628

D141 -0.00578 0.00001 0.00160 0.00144 0.00304 -0.00274

D142 -3.13266 -0.00004 0.00083 -0.00143 -0.00060 -3.13326

D143 3.12959 0.00005 0.00071 0.00275 0.00346 3.13306

D144 0.00272 -0.00000 -0.00006 -0.00012 -0.00018 0.00254

D145 -0.00144 0.00001 0.00084 0.00067 0.00151 0.00007

D146 3.13163 0.00003 -0.00002 0.00167 0.00165 3.13328

D147 -3.14121 0.00000 0.00082 0.00066 0.00147 -3.13974

D148 -0.00815 0.00003 -0.00004 0.00165 0.00161 -0.00654

D149 -0.00035 0.00001 0.00081 0.00086 0.00166 0.00131

D150 3.13501 0.00004 -0.00008 0.00217 0.00208 3.13709

D151 3.13942 0.00001 0.00083 0.00088 0.00170 3.14113

D152 -0.00840 0.00004 -0.00006 0.00218 0.00212 -0.00628

D153 -0.00217 -0.00001 -0.00171 -0.00167 -0.00338 -0.00555

D154 3.12622 0.00001 -0.00064 0.00021 -0.00044 3.12578

D155 -3.13526 -0.00004 -0.00086 -0.00267 -0.00353 -3.13879

D156 -0.00687 -0.00002 0.00021 -0.00079 -0.00059 -0.00746

D157 -3.13745 -0.00002 0.00097 -0.00079 0.00018 -3.13727

D158 0.00737 0.00001 0.00091 0.00109 0.00200 0.00937

D159 0.01726 -0.00005 -0.00009 -0.00264 -0.00273 0.01452

D160 -3.12110 -0.00001 -0.00015 -0.00076 -0.00091 -3.12202

D161 3.13563 0.00003 0.00068 0.00232 0.00300 3.13863

D162 0.00866 -0.00001 -0.00009 -0.00051 -0.00061 0.00805

D163 -0.00917 0.00000 0.00075 0.00045 0.00120 -0.00797

D164 -3.13614 -0.00004 -0.00003 -0.00238 -0.00241 -3.13856

D165 0.00578 -0.00001 -0.00160 -0.00144 -0.00304 0.00274

D166 -3.12959 -0.00005 -0.00071 -0.00275 -0.00346 -3.13306

D167 3.13266 0.00004 -0.00083 0.00143 0.00060 3.13326

D168 -0.00272 0.00000 0.00006 0.00012 0.00018 -0.00254

D169 3.13324 0.00005 0.00069 0.00314 0.00383 3.13707

D170 0.00721 -0.00001 -0.00010 0.00000 -0.00010 0.00711

D171 -0.00935 0.00000 0.00074 0.00023 0.00097 -0.00839

D172 -3.13538 -0.00005 -0.00004 -0.00291 -0.00296 -3.13834

D173 -3.13505 -0.00003 0.00098 -0.00159 -0.00061 -3.13566

D174 0.01946 -0.00005 -0.00010 -0.00324 -0.00334 0.01612

D175 0.00755 0.00001 0.00093 0.00134 0.00227 0.00982

D176 -3.12113 -0.00001 -0.00015 -0.00030 -0.00045 -3.12158

D177 0.00587 -0.00001 -0.00161 -0.00136 -0.00297 0.00290

D178 -3.12923 -0.00005 -0.00072 -0.00283 -0.00355 -3.13278

D179 3.13180 0.00004 -0.00082 0.00181 0.00098 3.13279

D180 -0.00330 0.00000 0.00007 0.00034 0.00040 -0.00290

D181 -0.00034 0.00001 0.00082 0.00092 0.00173 0.00138

D182 3.13953 0.00001 0.00083 0.00085 0.00167 3.14120

D183 3.13474 0.00004 -0.00008 0.00238 0.00230 3.13704

D184 -0.00857 0.00005 -0.00006 0.00232 0.00225 -0.00632

D185 -0.00144 0.00001 0.00085 0.00064 0.00148 0.00004

D186 3.13156 0.00003 -0.00002 0.00161 0.00159 3.13315

D187 -3.14131 0.00001 0.00083 0.00071 0.00154 -3.13978

D188 -0.00831 0.00003 -0.00003 0.00168 0.00164 -0.00667

D189 -0.00227 -0.00002 -0.00173 -0.00179 -0.00352 -0.00579

D190 3.12633 0.00001 -0.00065 -0.00012 -0.00077 3.12556

D191 -3.13530 -0.00005 -0.00087 -0.00277 -0.00364 -3.13894

D192 -0.00670 -0.00002 0.00021 -0.00110 -0.00089 -0.00759

D193 -3.13324 -0.00005 -0.00069 -0.00314 -0.00383 -3.13707

D194 -0.00721 0.00001 0.00010 -0.00000 0.00010 -0.00711

D195 0.00935 -0.00000 -0.00074 -0.00023 -0.00097 0.00839

D196 3.13538 0.00005 0.00004 0.00291 0.00296 3.13834

D197 3.13505 0.00003 -0.00098 0.00159 0.00061 3.13566

D198 -0.01946 0.00005 0.00010 0.00324 0.00334 -0.01612

D199 -0.00755 -0.00001 -0.00093 -0.00134 -0.00227 -0.00982

D200 3.12113 0.00001 0.00015 0.00030 0.00045 3.12158

D201 -0.00587 0.00001 0.00161 0.00136 0.00297 -0.00290

D202 3.12923 0.00005 0.00072 0.00283 0.00355 3.13278

D203 -3.13180 -0.00004 0.00082 -0.00181 -0.00098 -3.13279

D204 0.00330 -0.00000 -0.00007 -0.00034 -0.00040 0.00290

D205 0.00034 -0.00001 -0.00082 -0.00092 -0.00173 -0.00138

D206 -3.13953 -0.00001 -0.00083 -0.00085 -0.00167 -3.14120

D207 -3.13474 -0.00004 0.00008 -0.00238 -0.00230 -3.13704

D208 0.00857 -0.00005 0.00006 -0.00232 -0.00225 0.00632

D209 0.00144 -0.00001 -0.00085 -0.00064 -0.00148 -0.00004

D210 -3.13156 -0.00003 0.00002 -0.00161 -0.00159 -3.13315

D211 3.14131 -0.00001 -0.00083 -0.00071 -0.00154 3.13978

D212 0.00831 -0.00003 0.00003 -0.00168 -0.00164 0.00667

D213 0.00227 0.00002 0.00173 0.00179 0.00352 0.00579

D214 -3.12633 -0.00001 0.00065 0.00012 0.00077 -3.12556

D215 3.13530 0.00005 0.00087 0.00277 0.00364 3.13894

D216 0.00670 0.00002 -0.00021 0.00110 0.00089 0.00759

Item Value Threshold Converged?

Maximum Force 0.002335 0.000450 NO

RMS Force 0.000446 0.000300 NO

Maximum Displacement 0.249883 0.001800 NO

RMS Displacement 0.055138 0.001200 NO

Predicted change in Energy=-3.783421D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Aug 18 14:01:26 2019, MaxMem= 2013265920 cpu: 1.4

(Enter /home/kira/g09/l202.exe)

Stoichiometry C44H30N4(1-,2)

Framework group CS[SG(H2N2),X(C44H28N2)]

Deg. of freedom 116

Full point group CS NOp 2

RotChk: IX=3 Diff= 2.21D-04

Largest Abelian subgroup CS NOp 2

Largest concise Abelian subgroup CS NOp 2

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 4.247546 -0.251260 0.681164

2 6 0 2.895194 -0.049638 1.143163

3 7 0 2.117348 0.051229 -0.000000

4 6 0 2.895194 -0.049638 -1.143163

5 6 0 4.247546 -0.251260 -0.681164

6 6 0 2.460830 0.034413 -2.456060

7 6 0 1.095523 0.156066 -2.867440

8 7 0 0.000277 0.012025 -2.052729

9 6 0 -1.094717 0.158250 -2.867420

10 6 0 -0.687263 0.427584 -4.219074

11 6 0 0.688690 0.426291 -4.219113

12 6 0 2.460830 0.034413 2.456060

13 6 0 1.095523 0.156066 2.867440

14 6 0 0.688690 0.426291 4.219113

15 6 0 -0.687263 0.427584 4.219074

16 6 0 -1.094717 0.158250 2.867420

17 7 0 0.000277 0.012025 2.052729

18 6 0 -2.460375 0.038131 2.456364

19 6 0 -2.894965 -0.044423 1.143214

20 6 0 -4.246236 -0.252886 0.681165

21 6 0 -4.246236 -0.252886 -0.681165

22 6 0 -2.894965 -0.044423 -1.143214

23 7 0 -2.117725 0.059027 0.000000

24 6 0 -2.460375 0.038131 -2.456364

25 6 0 3.498645 -0.008827 -3.525383

26 6 0 4.520115 0.949477 -3.587791

27 6 0 5.490315 0.900387 -4.587143

28 6 0 5.454728 -0.106415 -5.550310

29 6 0 4.440541 -1.063479 -5.505101

30 6 0 3.473755 -1.012941 -4.504800

31 6 0 5.454728 -0.106415 5.550310

32 6 0 5.490315 0.900387 4.587143

33 6 0 4.520115 0.949477 3.587791

34 6 0 3.498645 -0.008827 3.525383

35 6 0 3.473755 -1.012941 4.504800

36 6 0 4.440541 -1.063479 5.505101

37 6 0 -3.498148 -0.006900 -3.525320

38 6 0 -3.469227 -1.008396 -4.507505

39 6 0 -4.437075 -1.061742 -5.506557

40 6 0 -5.456547 -0.110112 -5.548114

41 6 0 -5.496169 0.894163 -4.582487

42 6 0 -4.524871 0.946154 -3.584378

43 6 0 -3.498148 -0.006900 3.525320

44 6 0 -3.469227 -1.008396 4.507505

45 6 0 -4.437075 -1.061742 5.506557

46 6 0 -5.456547 -0.110112 5.548114

47 6 0 -5.496169 0.894163 4.582487

48 6 0 -4.524871 0.946154 3.584378

49 1 0 5.100044 -0.395013 1.326236

50 1 0 5.100044 -0.395013 -1.326236

51 1 0 -1.341474 0.609673 -5.059340

52 1 0 1.343206 0.606995 -5.059440

53 1 0 1.343206 0.606995 5.059440

54 1 0 -1.341474 0.609673 5.059340

55 1 0 -5.097673 -0.402706 1.326234

56 1 0 -5.097673 -0.402706 -1.326234

57 1 0 4.545756 1.744429 -2.850415

58 1 0 6.270049 1.654855 -4.616808

59 1 0 6.208519 -0.144737 -6.329908

60 1 0 4.405545 -1.854409 -6.247603

61 1 0 2.692985 -1.764827 -4.471525

62 1 0 6.208519 -0.144737 6.329908

63 1 0 6.270049 1.654855 4.616808

64 1 0 4.545756 1.744429 2.850415

65 1 0 2.692985 -1.764827 4.471525

66 1 0 4.405545 -1.854409 6.247603

67 1 0 -2.684688 -1.756419 -4.477002

68 1 0 -4.398835 -1.850753 -6.250942

69 1 0 -6.211230 -0.150687 -6.326730

70 1 0 -6.279952 1.644531 -4.609303

71 1 0 -4.553781 1.739371 -2.845284

72 1 0 -2.684688 -1.756419 4.477002

73 1 0 -4.398835 -1.850753 6.250942

74 1 0 -6.211230 -0.150687 6.326730

75 1 0 -6.279952 1.644531 4.609303

76 1 0 -4.553781 1.739371 2.845284

77 1 0 1.108791 0.113972 -0.000000

78 1 0 -1.110452 0.138530 0.000000

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

Rotational constants (GHZ): 0.0587302 0.0577491 0.0299836

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(Enter /home/kira/g09/l301.exe)

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

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

There are 513 symmetry adapted cartesian basis functions of A' symmetry.

There are 489 symmetry adapted cartesian basis functions of A" symmetry.

There are 488 symmetry adapted basis functions of A' symmetry.

There are 466 symmetry adapted basis functions of A" symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 161 beta electrons

nuclear repulsion energy 5349.4852982574 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= 78 NActive= 78 NUniq= 41 SFac= 3.62D+00 NAtFMM= 60 NAOKFM=T 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= -0.2121568439 Hartrees.

Nuclear repulsion after empirical dispersion term = 5349.2731414135 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= 78.

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

Smoothing algorithm: York/Karplus (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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5746

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.15D-11

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 246

GePol: Fraction of low-weight points (<1% of avg) = 4.28%

GePol: Cavity surface area = 613.461 Ang\*\*2

GePol: Cavity volume = 627.356 Ang\*\*3

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

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

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PCM non-electrostatic energy = -0.0020866270 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5349.2710547865 Hartrees.

Leave Link 301 at Sun Aug 18 14:01:26 2019, MaxMem= 2013265920 cpu: 1.0

(Enter /home/kira/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.

One-electron integral symmetry used in STVInt

NBasis= 954 RedAO= T EigKep= 9.11D-05 NBF= 488 466

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 488 466

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= 939 939 940 940 940 MxSgAt= 78 MxSgA2= 78.

Leave Link 302 at Sun Aug 18 14:01:27 2019, MaxMem= 2013265920 cpu: 11.1

(Enter /home/kira/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sun Aug 18 14:01:27 2019, MaxMem= 2013265920 cpu: 1.3

(Enter /home/kira/g09/l401.exe)

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

B after Tr= -0.000000 -0.000000 -0.000000

Rot= 1.000000 -0.000000 -0.000000 0.000023 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

Occupied (A') (A') (A") (A') (A') (A") (A') (A") (A") (A')

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The electronic state of the initial guess is 2-A'.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7586 S= 0.5043

Generating alternative initial guess.

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2000

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= -1914.57805028621

Leave Link 401 at Sun Aug 18 14:01:33 2019, MaxMem= 2013265920 cpu: 47.5

(Enter /home/kira/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3047318 IEndB= 3047318 NGot= 2013265920 MDV= 2011240249

LenX= 2011240249 LenY= 2010235243

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= 480000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 99049548.

Iteration 1 A\*A^-1 deviation from unit magnitude is 9.77D-15 for 5742.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.84D-15 for 3111 2879.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.88D-15 for 5742.

Iteration 1 A^-1\*A deviation from orthogonality is 6.97D-10 for 5517 3656.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.66D-15 for 2715.

Iteration 2 A\*A^-1 deviation from orthogonality is 3.23D-15 for 3587 350.

Iteration 2 A^-1\*A deviation from unit magnitude is 8.88D-16 for 639.

Iteration 2 A^-1\*A deviation from orthogonality is 3.47D-16 for 4431 4268.

E= -1914.47149038818

DIIS: error= 3.60D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.47149038818 IErMin= 1 ErrMin= 3.60D-03

ErrMax= 3.60D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.07D-02 BMatP= 4.07D-02

IDIUse=3 WtCom= 9.64D-01 WtEn= 3.60D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.446 Goal= None Shift= 0.000

Gap= 0.503 Goal= None Shift= 0.000

GapD= 0.446 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=1.46D-04 MaxDP=4.37D-03 OVMax= 2.04D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.46D-04 CP: 1.00D+00

E= -1914.49252542025 Delta-E= -0.021035032070 Rises=F Damp=F

DIIS: error= 5.11D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.49252542025 IErMin= 2 ErrMin= 5.11D-04

ErrMax= 5.11D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.12D-04 BMatP= 4.07D-02

IDIUse=3 WtCom= 9.95D-01 WtEn= 5.11D-03

Coeff-Com: -0.661D-01 0.107D+01

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

Coeff: -0.657D-01 0.107D+01

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=2.84D-05 MaxDP=8.49D-04 DE=-2.10D-02 OVMax= 3.84D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.50D-05 CP: 1.00D+00 1.09D+00

E= -1914.49281873250 Delta-E= -0.000293312256 Rises=F Damp=F

DIIS: error= 2.64D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.49281873250 IErMin= 3 ErrMin= 2.64D-04

ErrMax= 2.64D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.17D-04 BMatP= 6.12D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 2.64D-03

Coeff-Com: -0.366D-01 0.477D+00 0.560D+00

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

Coeff: -0.365D-01 0.475D+00 0.561D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.25D-05 MaxDP=8.19D-04 DE=-2.93D-04 OVMax= 2.78D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.03D-05 CP: 1.00D+00 1.10D+00 7.24D-01

E= -1914.49287453738 Delta-E= -0.000055804880 Rises=F Damp=F

DIIS: error= 1.40D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.49287453738 IErMin= 4 ErrMin= 1.40D-04

ErrMax= 1.40D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.50D-05 BMatP= 3.17D-04

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.40D-03

Coeff-Com: -0.978D-02 0.982D-01 0.343D+00 0.568D+00

Coeff-En: 0.000D+00 0.000D+00 0.219D+00 0.781D+00

Coeff: -0.977D-02 0.980D-01 0.343D+00 0.569D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=5.59D-06 MaxDP=3.14D-04 DE=-5.58D-05 OVMax= 1.33D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.30D-06 CP: 1.00D+00 1.11D+00 8.09D-01 6.27D-01

E= -1914.49289380236 Delta-E= -0.000019264982 Rises=F Damp=F

DIIS: error= 3.70D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.49289380236 IErMin= 5 ErrMin= 3.70D-05

ErrMax= 3.70D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.11D-06 BMatP= 8.50D-05

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

Coeff-Com: -0.135D-02 0.158D-02 0.103D+00 0.252D+00 0.645D+00

Coeff: -0.135D-02 0.158D-02 0.103D+00 0.252D+00 0.645D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.82D-06 MaxDP=1.26D-04 DE=-1.93D-05 OVMax= 3.77D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.27D-06 CP: 1.00D+00 1.11D+00 8.11D-01 7.15D-01 7.25D-01

E= -1914.49289453494 Delta-E= -0.000000732578 Rises=F Damp=F

DIIS: error= 2.21D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.49289453494 IErMin= 6 ErrMin= 2.21D-05

ErrMax= 2.21D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.36D-06 BMatP= 4.11D-06

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

Coeff-Com: 0.763D-03-0.158D-01 0.622D-02 0.620D-01 0.407D+00 0.540D+00

Coeff: 0.763D-03-0.158D-01 0.622D-02 0.620D-01 0.407D+00 0.540D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=7.73D-07 MaxDP=4.79D-05 DE=-7.33D-07 OVMax= 1.49D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.59D-07 CP: 1.00D+00 1.11D+00 8.23D-01 7.04D-01 8.00D-01

CP: 5.25D-01

E= -1914.49289486814 Delta-E= -0.000000333195 Rises=F Damp=F

DIIS: error= 3.09D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.49289486814 IErMin= 7 ErrMin= 3.09D-06

ErrMax= 3.09D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.94D-08 BMatP= 1.36D-06

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

Coeff-Com: 0.402D-03-0.769D-02 0.416D-03 0.240D-01 0.183D+00 0.266D+00

Coeff-Com: 0.534D+00

Coeff: 0.402D-03-0.769D-02 0.416D-03 0.240D-01 0.183D+00 0.266D+00

Coeff: 0.534D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.32D-07 MaxDP=6.27D-06 DE=-3.33D-07 OVMax= 2.62D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.11D-07 CP: 1.00D+00 1.11D+00 8.22D-01 7.07D-01 7.98D-01

CP: 5.67D-01 8.79D-01

E= -1914.49289487586 Delta-E= -0.000000007723 Rises=F Damp=F

DIIS: error= 1.91D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.49289487586 IErMin= 8 ErrMin= 1.91D-06

ErrMax= 1.91D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.85D-09 BMatP= 2.94D-08

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

Coeff-Com: -0.180D-04 0.763D-03-0.185D-02-0.630D-02-0.266D-01-0.202D-01

Coeff-Com: 0.277D+00 0.778D+00

Coeff: -0.180D-04 0.763D-03-0.185D-02-0.630D-02-0.266D-01-0.202D-01

Coeff: 0.277D+00 0.778D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=6.92D-08 MaxDP=3.61D-06 DE=-7.72D-09 OVMax= 1.94D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 4.96D-08 CP: 1.00D+00 1.11D+00 8.23D-01 7.06D-01 8.01D-01

CP: 5.66D-01 1.05D+00 9.79D-01

E= -1914.49289487887 Delta-E= -0.000000003009 Rises=F Damp=F

DIIS: error= 1.39D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.49289487887 IErMin= 9 ErrMin= 1.39D-06

ErrMax= 1.39D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.50D-09 BMatP= 5.85D-09

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

Coeff-Com: -0.718D-04 0.160D-02-0.963D-03-0.694D-02-0.424D-01-0.515D-01

Coeff-Com: 0.611D-01 0.403D+00 0.636D+00

Coeff: -0.718D-04 0.160D-02-0.963D-03-0.694D-02-0.424D-01-0.515D-01

Coeff: 0.611D-01 0.403D+00 0.636D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=3.71D-08 MaxDP=1.81D-06 DE=-3.01D-09 OVMax= 1.19D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 2.86D-08 CP: 1.00D+00 1.11D+00 8.23D-01 7.07D-01 8.01D-01

CP: 5.72D-01 1.11D+00 1.13D+00 9.90D-01

E= -1914.49289487970 Delta-E= -0.000000000830 Rises=F Damp=F

DIIS: error= 8.53D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.49289487970 IErMin=10 ErrMin= 8.53D-07

ErrMax= 8.53D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.34D-10 BMatP= 1.50D-09

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

Coeff-Com: -0.187D-04 0.235D-03 0.566D-03 0.403D-03-0.372D-02-0.100D-01

Coeff-Com: -0.109D+00-0.219D+00 0.271D+00 0.107D+01

Coeff: -0.187D-04 0.235D-03 0.566D-03 0.403D-03-0.372D-02-0.100D-01

Coeff: -0.109D+00-0.219D+00 0.271D+00 0.107D+01

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=3.56D-08 MaxDP=1.60D-06 DE=-8.30D-10 OVMax= 1.22D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.46D-08 CP: 1.00D+00 1.11D+00 8.23D-01 7.07D-01 8.02D-01

CP: 5.75D-01 1.17D+00 1.22D+00 1.48D+00 1.36D+00

E= -1914.49289488034 Delta-E= -0.000000000644 Rises=F Damp=F

DIIS: error= 3.63D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.49289488034 IErMin=11 ErrMin= 3.63D-07

ErrMax= 3.63D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.14D-10 BMatP= 4.34D-10

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

Coeff-Com: 0.960D-05-0.305D-03 0.532D-03 0.200D-02 0.910D-02 0.869D-02

Coeff-Com: -0.681D-01-0.206D+00-0.444D-01 0.520D+00 0.778D+00

Coeff: 0.960D-05-0.305D-03 0.532D-03 0.200D-02 0.910D-02 0.869D-02

Coeff: -0.681D-01-0.206D+00-0.444D-01 0.520D+00 0.778D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.59D-08 MaxDP=7.53D-07 DE=-6.44D-10 OVMax= 5.37D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 7.25D-09 CP: 1.00D+00 1.11D+00 8.23D-01 7.07D-01 8.02D-01

CP: 5.76D-01 1.18D+00 1.28D+00 1.66D+00 1.63D+00

CP: 1.09D+00

E= -1914.49289488051 Delta-E= -0.000000000164 Rises=F Damp=F

DIIS: error= 1.33D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.49289488051 IErMin=12 ErrMin= 1.33D-07

ErrMax= 1.33D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.54D-11 BMatP= 1.14D-10

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

Coeff-Com: 0.802D-05-0.187D-03 0.128D-03 0.839D-03 0.493D-02 0.610D-02

Coeff-Com: -0.954D-02-0.515D-01-0.797D-01 0.311D-01 0.352D+00 0.746D+00

Coeff: 0.802D-05-0.187D-03 0.128D-03 0.839D-03 0.493D-02 0.610D-02

Coeff: -0.954D-02-0.515D-01-0.797D-01 0.311D-01 0.352D+00 0.746D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=6.33D-09 MaxDP=3.07D-07 DE=-1.64D-10 OVMax= 2.08D-06

Error on total polarization charges = 0.08656

SCF Done: E(UB3LYP) = -1914.49289488 A.U. after 12 cycles

NFock= 12 Conv=0.63D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7586 S= 0.5043

<L.S>= 0.000000000000E+00

KE= 1.906555211164D+03 PE=-1.518336630473D+04 EE= 6.013047143899D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.31

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7586, after 0.7500

Leave Link 502 at Sun Aug 18 14:08:56 2019, MaxMem= 2013265920 cpu: 3523.8

(Enter /home/kira/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 = 185

Leave Link 701 at Sun Aug 18 14:09:14 2019, MaxMem= 2013265920 cpu: 139.6

(Enter /home/kira/g09/l702.exe)

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

Leave Link 702 at Sun Aug 18 14:09:14 2019, MaxMem= 2013265920 cpu: 0.1

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 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= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

Petite list used in FoFCou.

Leave Link 703 at Sun Aug 18 14:10:27 2019, MaxMem= 2013265920 cpu: 588.6

(Enter /home/kira/g09/l716.exe)

Dipole =-1.48964816D-03-1.45680162D-01-1.23101529D-12

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000114188 -0.000358085 -0.000329186

2 6 0.000722077 0.000360927 -0.001559941

3 7 0.000682265 -0.000520097 0.000000000

4 6 0.000722077 0.000360927 0.001559941

5 6 -0.000114188 -0.000358085 0.000329186

6 6 -0.000180484 -0.000156852 -0.000434542

7 6 -0.000337473 -0.000865927 -0.000766180

8 7 -0.000018452 0.001443936 -0.000542011

9 6 0.000310005 -0.000892994 -0.000794626

10 6 0.000104503 0.000344363 0.000144177

11 6 -0.000112451 0.000286606 0.000161253

12 6 -0.000180484 -0.000156852 0.000434542

13 6 -0.000337473 -0.000865927 0.000766180

14 6 -0.000112451 0.000286606 -0.000161253

15 6 0.000104503 0.000344363 -0.000144177

16 6 0.000310005 -0.000892994 0.000794626

17 7 -0.000018452 0.001443936 0.000542011

18 6 0.000205995 -0.000074779 0.000333552

19 6 -0.000687243 0.000181650 -0.001526583

20 6 0.000102505 -0.000322782 -0.000315706

21 6 0.000102505 -0.000322782 0.000315706

22 6 -0.000687243 0.000181650 0.001526583

23 7 -0.000675301 -0.000297410 -0.000000000

24 6 0.000205995 -0.000074779 -0.000333552

25 6 0.000695876 0.000252255 -0.000689838

26 6 -0.000298465 0.000092606 0.000284638

27 6 -0.000094109 0.000095216 -0.000162709

28 6 -0.000122261 -0.000020183 0.000111058

29 6 0.000143378 -0.000046191 0.000111096

30 6 -0.000205803 -0.000303089 0.000406348

31 6 -0.000122261 -0.000020183 -0.000111058

32 6 -0.000094109 0.000095216 0.000162709

33 6 -0.000298465 0.000092606 -0.000284638

34 6 0.000695876 0.000252255 0.000689838

35 6 -0.000205803 -0.000303089 -0.000406348

36 6 0.000143378 -0.000046191 -0.000111096

37 6 -0.000746862 0.000221884 -0.000760734

38 6 0.000192681 -0.000303279 0.000449558

39 6 -0.000145807 -0.000028020 0.000089427

40 6 0.000131688 -0.000031449 0.000117208

41 6 0.000093750 0.000102337 -0.000165678

42 6 0.000323405 0.000087259 0.000293934

43 6 -0.000746862 0.000221884 0.000760734

44 6 0.000192681 -0.000303279 -0.000449558

45 6 -0.000145807 -0.000028020 -0.000089427

46 6 0.000131688 -0.000031449 -0.000117208

47 6 0.000093750 0.000102337 0.000165678

48 6 0.000323405 0.000087259 -0.000293934

49 1 -0.000101726 0.000133863 -0.000056030

50 1 -0.000101726 0.000133863 0.000056030

51 1 0.000211500 -0.000012554 0.000231151

52 1 -0.000198474 -0.000023015 0.000230900

53 1 -0.000198474 -0.000023015 -0.000230900

54 1 0.000211500 -0.000012554 -0.000231151

55 1 0.000097214 0.000133588 -0.000058880

56 1 0.000097214 0.000133588 0.000058880

57 1 0.000044285 0.000048759 -0.000043093

58 1 -0.000077703 -0.000021175 0.000039790

59 1 -0.000022392 0.000000768 0.000029020

60 1 -0.000043979 0.000027069 0.000081770

61 1 0.000063725 -0.000029024 -0.000048643

62 1 -0.000022392 0.000000768 -0.000029020

63 1 -0.000077703 -0.000021175 -0.000039790

64 1 0.000044285 0.000048759 0.000043093

65 1 0.000063725 -0.000029024 0.000048643

66 1 -0.000043979 0.000027069 -0.000081770

67 1 -0.000061057 -0.000033987 -0.000045236

68 1 0.000045116 0.000029134 0.000080698

69 1 0.000021940 0.000000836 0.000029376

70 1 0.000077855 -0.000019308 0.000041554

71 1 -0.000049051 0.000048222 -0.000035522

72 1 -0.000061057 -0.000033987 0.000045236

73 1 0.000045116 0.000029134 -0.000080698

74 1 0.000021940 0.000000836 -0.000029376

75 1 0.000077855 -0.000019308 -0.000041554

76 1 -0.000049051 0.000048222 0.000035522

77 1 -0.000075619 0.000140207 -0.000000000

78 1 0.000129621 -0.000019865 0.000000000

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

Cartesian Forces: Max 0.001559941 RMS 0.000379254

Leave Link 716 at Sun Aug 18 14:10:27 2019, MaxMem= 2013265920 cpu: 0.2

(Enter /home/kira/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 0.001178309 RMS 0.000240533

Search for a local minimum.

Step number 3 out of a maximum of 452

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

RMS Force = .24053D-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= -4.14D-04 DEPred=-3.78D-04 R= 1.09D+00

TightC=F SS= 1.41D+00 RLast= 1.90D-01 DXNew= 8.4853D-01 5.7022D-01

Trust test= 1.09D+00 RLast= 1.90D-01 DXMaxT set to 5.70D-01

ITU= 1 1 0

Eigenvalues --- 0.00416 0.00983 0.00985 0.00988 0.01504

Eigenvalues --- 0.01614 0.01616 0.01619 0.01646 0.01660

Eigenvalues --- 0.01721 0.01721 0.01721 0.01722 0.01731

Eigenvalues --- 0.01742 0.01752 0.01783 0.01788 0.01797

Eigenvalues --- 0.01836 0.01854 0.01855 0.01891 0.01893

Eigenvalues --- 0.01903 0.01930 0.01944 0.01980 0.01988

Eigenvalues --- 0.02006 0.02011 0.02021 0.02027 0.02048

Eigenvalues --- 0.02068 0.02069 0.02070 0.02070 0.02080

Eigenvalues --- 0.02104 0.02106 0.02118 0.02118 0.02119

Eigenvalues --- 0.02119 0.02130 0.02132 0.02132 0.02132

Eigenvalues --- 0.02132 0.02132 0.02160 0.02160 0.02160

Eigenvalues --- 0.02160 0.02162 0.02162 0.02162 0.02173

Eigenvalues --- 0.02173 0.02173 0.02173 0.02181 0.02181

Eigenvalues --- 0.02181 0.02181 0.02186 0.02186 0.02187

Eigenvalues --- 0.02187 0.02210 0.02216 0.02217 0.02821

Eigenvalues --- 0.15924 0.15951 0.15993 0.15994 0.15995

Eigenvalues --- 0.15996 0.15996 0.15997 0.15998 0.15998

Eigenvalues --- 0.15999 0.15999 0.15999 0.15999 0.15999

Eigenvalues --- 0.15999 0.15999 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16001 0.16023

Eigenvalues --- 0.22000 0.22000 0.22000 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22004 0.22752 0.22768

Eigenvalues --- 0.22808 0.22825 0.23469 0.23469 0.23469

Eigenvalues --- 0.23538 0.23578 0.24272 0.24436 0.24678

Eigenvalues --- 0.24756 0.24862 0.24959 0.24986 0.24995

Eigenvalues --- 0.24997 0.24999 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.26261 0.28411 0.34159 0.34181 0.34206

Eigenvalues --- 0.34569 0.35413 0.35413 0.35413 0.35414

Eigenvalues --- 0.35415 0.35415 0.35416 0.35416 0.35416

Eigenvalues --- 0.35416 0.35416 0.35446 0.35506 0.35507

Eigenvalues --- 0.35508 0.35524 0.35542 0.35544 0.35547

Eigenvalues --- 0.35656 0.36056 0.36057 0.36058 0.36112

Eigenvalues --- 0.36250 0.36250 0.36251 0.36274 0.37121

Eigenvalues --- 0.37161 0.37254 0.37288 0.39062 0.39127

Eigenvalues --- 0.39740 0.40035 0.40243 0.40418 0.40454

Eigenvalues --- 0.40924 0.41796 0.41803 0.41811 0.42077

Eigenvalues --- 0.42078 0.42082 0.42082 0.42170 0.43258

Eigenvalues --- 0.44083 0.44661 0.45342 0.45570 0.45571

Eigenvalues --- 0.45586 0.45588 0.45681 0.45769 0.45845

Eigenvalues --- 0.45904 0.45930 0.45938 0.45942 0.45944

Eigenvalues --- 0.45963 0.46660 0.46661 0.46661 0.46667

Eigenvalues --- 0.47073 0.47079 0.47086 0.47428 0.48184

Eigenvalues --- 0.48277 0.49328 0.49423 0.49515 0.49969

Eigenvalues --- 0.50804 0.51674 0.54515

En-DIIS/RFO-DIIS IScMMF= 0 using points: 3 2

RFO step: Lambda=-9.15453436D-05.

NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=F DC= 4.14D-04 SmlDif= 1.00D-05

RMS Error= 0.1405319842D-02 NUsed= 2 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.17124 -0.17124

Iteration 1 RMS(Cart)= 0.12410355 RMS(Int)= 0.00418441

Iteration 2 RMS(Cart)= 0.00912952 RMS(Int)= 0.00019340

Iteration 3 RMS(Cart)= 0.00004964 RMS(Int)= 0.00019277

Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00019277

ITry= 1 IFail=0 DXMaxC= 3.94D-01 DCOld= 1.00D+10 DXMaxT= 5.70D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 4.36D-08 for atom 56.

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

(Linear) (Quad) (Total)

R1 2.72733 -0.00020 0.00101 0.00627 0.00736 2.73469

R2 2.57443 -0.00047 -0.00103 -0.00720 -0.00799 2.56644

R3 2.03840 -0.00013 0.00009 0.00024 0.00034 2.03873

R4 2.61987 -0.00060 0.00067 0.00416 0.00464 2.62451

R5 2.61810 0.00118 -0.00150 -0.00770 -0.00918 2.60891

R6 2.61987 -0.00060 0.00067 0.00416 0.00464 2.62451

R7 1.90958 0.00008 0.00013 0.00057 0.00070 1.91028

R8 2.72733 -0.00020 0.00101 0.00627 0.00736 2.73469

R9 2.61810 0.00118 -0.00150 -0.00770 -0.00918 2.60891

R10 2.03840 -0.00013 0.00009 0.00024 0.00034 2.03873

R11 2.70442 0.00088 -0.00047 -0.00033 -0.00080 2.70362

R12 2.81714 -0.00003 0.00028 0.00341 0.00369 2.82083

R13 2.59386 -0.00019 -0.00019 -0.00072 -0.00114 2.59272

R14 2.71592 -0.00023 0.00050 0.00297 0.00355 2.71947

R15 2.59390 -0.00020 -0.00018 -0.00070 -0.00109 2.59280

R16 2.71590 -0.00021 0.00052 0.00316 0.00375 2.71966

R17 2.70463 0.00085 -0.00050 -0.00057 -0.00107 2.70356

R18 2.60017 0.00000 -0.00061 -0.00324 -0.00358 2.59660

R19 2.04160 -0.00031 0.00007 -0.00042 -0.00035 2.04125

R20 2.04160 -0.00030 0.00008 -0.00037 -0.00029 2.04131

R21 2.70442 0.00088 -0.00047 -0.00033 -0.00080 2.70362

R22 2.81714 -0.00003 0.00028 0.00341 0.00369 2.82083

R23 2.71592 -0.00023 0.00050 0.00297 0.00355 2.71947

R24 2.59386 -0.00019 -0.00019 -0.00072 -0.00114 2.59272

R25 2.60017 0.00000 -0.00061 -0.00324 -0.00358 2.59660

R26 2.04160 -0.00030 0.00008 -0.00037 -0.00029 2.04131

R27 2.71590 -0.00021 0.00052 0.00316 0.00375 2.71966

R28 2.04160 -0.00031 0.00007 -0.00042 -0.00035 2.04125

R29 2.59390 -0.00020 -0.00018 -0.00070 -0.00109 2.59280

R30 2.70463 0.00085 -0.00050 -0.00057 -0.00107 2.70356

R31 2.61851 0.00112 -0.00147 -0.00770 -0.00919 2.60932

R32 2.81669 0.00001 0.00032 0.00380 0.00412 2.82081

R33 2.72729 -0.00019 0.00103 0.00640 0.00751 2.73480

R34 2.61967 -0.00058 0.00068 0.00426 0.00472 2.62439

R35 2.57443 -0.00048 -0.00105 -0.00731 -0.00810 2.56633

R36 2.03837 -0.00013 0.00009 0.00021 0.00030 2.03867

R37 2.72729 -0.00019 0.00103 0.00640 0.00751 2.73480

R38 2.03837 -0.00013 0.00009 0.00021 0.00030 2.03867

R39 2.61967 -0.00058 0.00068 0.00426 0.00472 2.62439

R40 2.61851 0.00112 -0.00147 -0.00770 -0.00919 2.60932

R41 1.90939 0.00013 0.00017 0.00094 0.00111 1.91050

R42 2.81669 0.00001 0.00032 0.00380 0.00412 2.82081

R43 2.64942 -0.00026 -0.00020 -0.00173 -0.00194 2.64748

R44 2.65109 -0.00021 -0.00021 -0.00157 -0.00178 2.64931

R45 2.63371 -0.00013 -0.00006 -0.00017 -0.00023 2.63348

R46 2.04957 0.00001 0.00014 0.00085 0.00099 2.05056

R47 2.63385 -0.00000 0.00007 0.00031 0.00038 2.63424

R48 2.05110 -0.00007 0.00002 -0.00000 0.00001 2.05112

R49 2.63655 -0.00003 0.00006 0.00017 0.00023 2.63678

R50 2.05054 -0.00004 -0.00002 -0.00013 -0.00014 2.05040

R51 2.63061 -0.00017 -0.00008 -0.00038 -0.00046 2.63015

R52 2.05112 -0.00007 0.00001 -0.00003 -0.00002 2.05110

R53 2.04932 -0.00003 0.00017 0.00091 0.00108 2.05040

R54 2.63385 -0.00000 0.00007 0.00031 0.00038 2.63424

R55 2.63655 -0.00003 0.00006 0.00017 0.00023 2.63678

R56 2.05054 -0.00004 -0.00002 -0.00013 -0.00014 2.05040

R57 2.63371 -0.00013 -0.00006 -0.00017 -0.00023 2.63348

R58 2.05110 -0.00007 0.00002 -0.00000 0.00001 2.05112

R59 2.64942 -0.00026 -0.00020 -0.00173 -0.00194 2.64748

R60 2.04957 0.00001 0.00014 0.00085 0.00099 2.05056

R61 2.65109 -0.00021 -0.00021 -0.00157 -0.00178 2.64931

R62 2.63061 -0.00017 -0.00008 -0.00038 -0.00046 2.63015

R63 2.04932 -0.00003 0.00017 0.00091 0.00108 2.05040

R64 2.05112 -0.00007 0.00001 -0.00003 -0.00002 2.05110

R65 2.65136 -0.00024 -0.00022 -0.00170 -0.00192 2.64944

R66 2.64964 -0.00028 -0.00021 -0.00181 -0.00202 2.64762

R67 2.63051 -0.00016 -0.00007 -0.00032 -0.00038 2.63013

R68 2.04926 -0.00002 0.00017 0.00094 0.00111 2.05037

R69 2.63659 -0.00004 0.00005 0.00015 0.00020 2.63679

R70 2.05112 -0.00008 0.00001 -0.00003 -0.00002 2.05110

R71 2.63383 -0.00000 0.00007 0.00030 0.00037 2.63420

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A1 1.89664 -0.00006 0.00019 0.00184 0.00192 1.89856

A2 2.17455 0.00000 -0.00006 -0.00095 -0.00095 2.17360

A3 2.21183 0.00006 -0.00013 -0.00087 -0.00095 2.21088

A4 1.84620 0.00003 0.00003 -0.00143 -0.00150 1.84471

A5 2.22132 0.00005 -0.00015 -0.00080 -0.00024 2.22108

A6 2.21564 -0.00008 0.00011 0.00231 0.00173 2.21737

A7 1.93888 0.00005 -0.00033 -0.00036 -0.00066 1.93822

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A16 2.18544 0.00049 0.00028 0.00369 0.00300 2.18844

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A19 2.19161 -0.00003 0.00038 0.00489 0.00448 2.19609

A20 2.16083 0.00047 -0.00088 -0.00381 -0.00403 2.15679

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A22 1.84738 0.00057 -0.00053 0.00069 0.00044 1.84782

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A25 2.16079 0.00051 -0.00086 -0.00352 -0.00371 2.15709

A26 1.85809 0.00013 -0.00015 0.00025 0.00005 1.85814

A27 2.20356 -0.00003 0.00012 0.00032 0.00046 2.20402

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D3 -3.11185 0.00001 -0.00238 -0.01356 -0.01595 -3.12780

D4 0.03586 -0.00022 -0.00198 -0.02683 -0.02882 0.00704

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D7 3.12254 -0.00002 0.00024 0.00111 0.00134 3.12388

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D91 2.11134 -0.00053 -0.00344 -0.08622 -0.08966 2.02168

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D104 -0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D105 0.01219 -0.00001 -0.00198 -0.01090 -0.01290 -0.00071

D106 -3.12769 -0.00020 -0.00117 -0.01935 -0.02056 3.13494

D107 -3.10885 -0.00000 -0.00235 -0.01381 -0.01616 -3.12501

D108 0.03446 -0.00019 -0.00154 -0.02226 -0.02382 0.01064

D109 -0.02042 0.00002 0.00333 0.01828 0.02161 0.00119

D110 3.05626 -0.00011 -0.00024 -0.01078 -0.01102 3.04524

D111 3.11947 0.00021 0.00252 0.02670 0.02924 -3.13447

D112 -0.08704 0.00008 -0.00104 -0.00236 -0.00339 -0.09042

D113 -3.06557 0.00006 -0.00456 -0.02561 -0.03016 -3.09573

D114 0.07185 0.00005 -0.00534 -0.03052 -0.03586 0.03599

D115 0.07808 -0.00017 -0.00359 -0.03579 -0.03939 0.03869

D116 -3.06768 -0.00018 -0.00437 -0.04069 -0.04509 -3.11277

D117 1.02641 0.00052 0.00272 0.08172 0.08444 1.11085

D118 -2.11119 0.00045 0.00322 0.07993 0.08315 -2.02804

D119 -2.11134 0.00053 0.00344 0.08622 0.08966 -2.02168

D120 1.03424 0.00046 0.00394 0.08443 0.08837 1.12261

D121 3.13727 0.00002 -0.00003 -0.00088 -0.00092 3.13636

D122 -0.01452 -0.00006 0.00047 -0.00150 -0.00103 -0.01556

D123 -0.00937 0.00009 -0.00034 0.00228 0.00194 -0.00743

D124 3.12202 0.00000 0.00016 0.00167 0.00183 3.12384

D125 -3.13863 0.00008 -0.00051 0.00127 0.00075 -3.13788

D126 -0.00805 0.00002 0.00010 0.00219 0.00229 -0.00576

D127 0.00797 0.00001 -0.00020 -0.00188 -0.00209 0.00589

D128 3.13856 -0.00005 0.00041 -0.00096 -0.00055 3.13801

D129 0.00555 -0.00012 0.00058 -0.00136 -0.00078 0.00477

D130 3.13879 -0.00006 0.00060 0.00102 0.00163 3.14042

D131 -3.12578 -0.00003 0.00007 -0.00075 -0.00068 -3.12646

D132 0.00746 0.00002 0.00010 0.00163 0.00173 0.00919

D133 -0.00007 0.00004 -0.00026 -0.00002 -0.00028 -0.00035

D134 3.13974 0.00005 -0.00025 0.00062 0.00037 3.14011

D135 -3.13328 -0.00001 -0.00028 -0.00241 -0.00269 -3.13597

D136 0.00654 -0.00000 -0.00028 -0.00177 -0.00205 0.00449

D137 -0.00131 0.00005 -0.00029 0.00042 0.00014 -0.00118

D138 -3.13709 0.00001 -0.00036 -0.00134 -0.00170 -3.13879

D139 -3.14113 0.00004 -0.00029 -0.00022 -0.00051 3.14155

D140 0.00628 -0.00000 -0.00036 -0.00198 -0.00234 0.00393

D141 -0.00274 -0.00008 0.00052 0.00056 0.00108 -0.00166

D142 -3.13326 -0.00002 -0.00010 -0.00038 -0.00048 -3.13374

D143 3.13306 -0.00003 0.00059 0.00232 0.00291 3.13597

D144 0.00254 0.00003 -0.00003 0.00138 0.00135 0.00389

D145 0.00007 -0.00004 0.00026 0.00002 0.00028 0.00035

D146 3.13328 0.00001 0.00028 0.00241 0.00269 3.13597

D147 -3.13974 -0.00005 0.00025 -0.00062 -0.00037 -3.14011

D148 -0.00654 0.00000 0.00028 0.00177 0.00205 -0.00449

D149 0.00131 -0.00005 0.00029 -0.00042 -0.00014 0.00118

D150 3.13709 -0.00001 0.00036 0.00134 0.00170 3.13879

D151 3.14113 -0.00004 0.00029 0.00022 0.00051 -3.14155

D152 -0.00628 0.00000 0.00036 0.00198 0.00234 -0.00393

D153 -0.00555 0.00012 -0.00058 0.00136 0.00078 -0.00477

D154 3.12578 0.00003 -0.00007 0.00075 0.00068 3.12646

D155 -3.13879 0.00006 -0.00060 -0.00102 -0.00163 -3.14042

D156 -0.00746 -0.00002 -0.00010 -0.00163 -0.00173 -0.00919

D157 -3.13727 -0.00002 0.00003 0.00088 0.00092 -3.13636

D158 0.00937 -0.00009 0.00034 -0.00228 -0.00194 0.00743

D159 0.01452 0.00006 -0.00047 0.00150 0.00103 0.01556

D160 -3.12202 -0.00000 -0.00016 -0.00167 -0.00183 -3.12384

D161 3.13863 -0.00008 0.00051 -0.00127 -0.00075 3.13788

D162 0.00805 -0.00002 -0.00010 -0.00219 -0.00229 0.00576

D163 -0.00797 -0.00001 0.00020 0.00188 0.00209 -0.00589

D164 -3.13856 0.00005 -0.00041 0.00096 0.00055 -3.13801

D165 0.00274 0.00008 -0.00052 -0.00056 -0.00108 0.00166

D166 -3.13306 0.00003 -0.00059 -0.00232 -0.00291 -3.13597

D167 3.13326 0.00002 0.00010 0.00038 0.00048 3.13374

D168 -0.00254 -0.00003 0.00003 -0.00138 -0.00135 -0.00389

D169 3.13707 -0.00006 0.00066 0.00051 0.00117 3.13824

D170 0.00711 -0.00001 -0.00002 -0.00125 -0.00127 0.00585

D171 -0.00839 -0.00000 0.00017 0.00225 0.00241 -0.00597

D172 -3.13834 0.00005 -0.00051 0.00049 -0.00002 -3.13836

D173 -3.13566 -0.00003 -0.00010 -0.00057 -0.00068 -3.13633

D174 0.01612 0.00005 -0.00057 0.00030 -0.00027 0.01585

D175 0.00982 -0.00009 0.00039 -0.00232 -0.00193 0.00790

D176 -3.12158 -0.00001 -0.00008 -0.00145 -0.00153 -3.12311

D177 0.00290 0.00007 -0.00051 -0.00103 -0.00154 0.00136

D178 -3.13278 0.00003 -0.00061 -0.00279 -0.00340 -3.13618

D179 3.13279 0.00002 0.00017 0.00075 0.00092 3.13370

D180 -0.00290 -0.00003 0.00007 -0.00101 -0.00094 -0.00384

D181 0.00138 -0.00005 0.00030 -0.00018 0.00012 0.00151

D182 3.14120 -0.00004 0.00029 0.00035 0.00064 -3.14135

D183 3.13704 -0.00001 0.00039 0.00158 0.00198 3.13902

D184 -0.00632 0.00000 0.00039 0.00211 0.00249 -0.00383

D185 0.00004 -0.00004 0.00025 0.00010 0.00036 0.00040

D186 3.13315 0.00001 0.00027 0.00235 0.00263 3.13578

D187 -3.13978 -0.00005 0.00026 -0.00042 -0.00016 -3.13993

D188 -0.00667 0.00001 0.00028 0.00183 0.00211 -0.00455

D189 -0.00579 0.00012 -0.00060 0.00118 0.00057 -0.00522

D190 3.12556 0.00003 -0.00013 0.00031 0.00018 3.12574

D191 -3.13894 0.00006 -0.00062 -0.00107 -0.00169 -3.14063

D192 -0.00759 -0.00002 -0.00015 -0.00194 -0.00209 -0.00968

D193 -3.13707 0.00006 -0.00066 -0.00051 -0.00117 -3.13824

D194 -0.00711 0.00001 0.00002 0.00125 0.00127 -0.00585

D195 0.00839 0.00000 -0.00017 -0.00225 -0.00241 0.00597

D196 3.13834 -0.00005 0.00051 -0.00049 0.00002 3.13836

D197 3.13566 0.00003 0.00010 0.00057 0.00068 3.13633

D198 -0.01612 -0.00005 0.00057 -0.00030 0.00027 -0.01585

D199 -0.00982 0.00009 -0.00039 0.00232 0.00193 -0.00790

D200 3.12158 0.00001 0.00008 0.00145 0.00153 3.12311

D201 -0.00290 -0.00007 0.00051 0.00103 0.00154 -0.00136

D202 3.13278 -0.00003 0.00061 0.00279 0.00340 3.13618

D203 -3.13279 -0.00002 -0.00017 -0.00075 -0.00092 -3.13370

D204 0.00290 0.00003 -0.00007 0.00101 0.00094 0.00384

D205 -0.00138 0.00005 -0.00030 0.00018 -0.00012 -0.00151

D206 -3.14120 0.00004 -0.00029 -0.00035 -0.00064 3.14135

D207 -3.13704 0.00001 -0.00039 -0.00158 -0.00198 -3.13902

D208 0.00632 -0.00000 -0.00039 -0.00211 -0.00249 0.00383

D209 -0.00004 0.00004 -0.00025 -0.00010 -0.00036 -0.00040

D210 -3.13315 -0.00001 -0.00027 -0.00235 -0.00263 -3.13578

D211 3.13978 0.00005 -0.00026 0.00042 0.00016 3.13993

D212 0.00667 -0.00001 -0.00028 -0.00183 -0.00211 0.00455

D213 0.00579 -0.00012 0.00060 -0.00118 -0.00057 0.00522

D214 -3.12556 -0.00003 0.00013 -0.00031 -0.00018 -3.12574

D215 3.13894 -0.00006 0.00062 0.00107 0.00169 3.14063

D216 0.00759 0.00002 0.00015 0.00194 0.00209 0.00968

Item Value Threshold Converged?

Maximum Force 0.001178 0.000450 NO

RMS Force 0.000241 0.000300 YES

Maximum Displacement 0.394358 0.001800 NO

RMS Displacement 0.129430 0.001200 NO

Predicted change in Energy=-4.363383D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Aug 18 14:10:28 2019, MaxMem= 2013265920 cpu: 1.4

(Enter /home/kira/g09/l202.exe)

Stoichiometry C44H30N4(1-,2)

Framework group CS[SG(H2N2),X(C44H28N2)]

Deg. of freedom 116

Full point group CS NOp 2

RotChk: IX=3 Diff= 4.01D-04

Largest Abelian subgroup CS NOp 2

Largest concise Abelian subgroup CS NOp 2

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 4.263755 -0.098732 0.679050

2 6 0 2.899136 0.023660 1.144927

3 7 0 2.116575 0.098475 0.000000

4 6 0 2.899136 0.023660 -1.144927

5 6 0 4.263755 -0.098732 -0.679050

6 6 0 2.462281 0.051583 -2.454268

7 6 0 1.094978 0.117111 -2.870292

8 7 0 0.000197 0.025141 -2.048459

9 6 0 -1.094684 0.114228 -2.870544

10 6 0 -0.686859 0.297762 -4.238474

11 6 0 0.687199 0.299261 -4.238319

12 6 0 2.462281 0.051583 2.454268

13 6 0 1.094978 0.117111 2.870292

14 6 0 0.687199 0.299261 4.238319

15 6 0 -0.686859 0.297762 4.238474

16 6 0 -1.094684 0.114228 2.870544

17 7 0 0.000197 0.025141 2.048459

18 6 0 -2.461816 0.045735 2.454544

19 6 0 -2.898333 0.014167 1.144945

20 6 0 -4.263059 -0.107489 0.679021

21 6 0 -4.263059 -0.107489 -0.679021

22 6 0 -2.898333 0.014167 -1.144945

23 7 0 -2.115537 0.084906 -0.000000

24 6 0 -2.461816 0.045735 -2.454544

25 6 0 3.501096 -0.006317 -3.524651

26 6 0 4.438393 1.022270 -3.686665

27 6 0 5.409396 0.958709 -4.684247

28 6 0 5.458609 -0.135947 -5.545920

29 6 0 4.528310 -1.165588 -5.399926

30 6 0 3.561357 -1.098902 -4.401070

31 6 0 5.458609 -0.135947 5.545920

32 6 0 5.409396 0.958709 4.684247

33 6 0 4.438393 1.022270 3.686665

34 6 0 3.501096 -0.006317 3.524651

35 6 0 3.561357 -1.098902 4.401070

36 6 0 4.528310 -1.165588 5.399926

37 6 0 -3.501147 -0.008016 -3.524628

38 6 0 -3.559535 -1.095055 -4.408149

39 6 0 -4.526777 -1.157416 -5.406983

40 6 0 -5.459664 -0.129114 -5.545793

41 6 0 -5.412404 0.960056 -4.677117

42 6 0 -4.440837 1.019529 -3.679868

43 6 0 -3.501147 -0.008016 3.524628

44 6 0 -3.559535 -1.095055 4.408149

45 6 0 -4.526777 -1.157416 5.406983

46 6 0 -5.459664 -0.129114 5.545793

47 6 0 -5.412404 0.960056 4.677117

48 6 0 -4.440837 1.019529 3.679868

49 1 0 5.124080 -0.191278 1.323405

50 1 0 5.124080 -0.191278 -1.323405

51 1 0 -1.340695 0.425641 -5.088735

52 1 0 1.341122 0.428286 -5.088377

53 1 0 1.341122 0.428286 5.088377

54 1 0 -1.340695 0.425641 5.088735

55 1 0 -5.123490 -0.199620 1.323240

56 1 0 -5.123490 -0.199620 -1.323240

57 1 0 4.398202 1.884529 -3.029124

58 1 0 6.123786 1.768977 -4.790160

59 1 0 6.213049 -0.186502 -6.324085

60 1 0 4.557393 -2.024669 -6.062655

61 1 0 2.846318 -1.907374 -4.289843

62 1 0 6.213049 -0.186502 6.324085

63 1 0 6.123786 1.768977 4.790160

64 1 0 4.398202 1.884529 3.029124

65 1 0 2.846318 -1.907374 4.289843

66 1 0 4.557393 -2.024669 6.062655

67 1 0 -2.842577 -1.902575 -4.302670

68 1 0 -4.554102 -2.012209 -6.075312

69 1 0 -6.214447 -0.176411 -6.323826

70 1 0 -6.128647 1.769411 -4.777381

71 1 0 -4.401935 1.878001 -3.017341

72 1 0 -2.842577 -1.902575 4.302670

73 1 0 -4.554102 -2.012209 6.075312

74 1 0 -6.214447 -0.176411 6.323826

75 1 0 -6.128647 1.769411 4.777381

76 1 0 -4.401935 1.878001 3.017341

77 1 0 1.105712 0.103349 0.000000

78 1 0 -1.104590 0.094632 -0.000000

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

Rotational constants (GHZ): 0.0585317 0.0576611 0.0300210

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(Enter /home/kira/g09/l301.exe)

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

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

There are 513 symmetry adapted cartesian basis functions of A' symmetry.

There are 489 symmetry adapted cartesian basis functions of A" symmetry.

There are 488 symmetry adapted basis functions of A' symmetry.

There are 466 symmetry adapted basis functions of A" symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 161 beta electrons

nuclear repulsion energy 5346.0705636229 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= 78 NActive= 78 NUniq= 41 SFac= 3.62D+00 NAtFMM= 60 NAOKFM=T 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= -0.2116743699 Hartrees.

Nuclear repulsion after empirical dispersion term = 5345.8588892530 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= 78.

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

Smoothing algorithm: York/Karplus (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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5714

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.27D-10

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 304

GePol: Fraction of low-weight points (<1% of avg) = 5.32%

GePol: Cavity surface area = 618.039 Ang\*\*2

GePol: Cavity volume = 629.793 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0019965268 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5345.8568927262 Hartrees.

Leave Link 301 at Sun Aug 18 14:10:28 2019, MaxMem= 2013265920 cpu: 1.1

(Enter /home/kira/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.

One-electron integral symmetry used in STVInt

NBasis= 954 RedAO= T EigKep= 9.00D-05 NBF= 488 466

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 488 466

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= 938 938 939 939 940 MxSgAt= 78 MxSgA2= 78.

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(Enter /home/kira/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sun Aug 18 14:10:29 2019, MaxMem= 2013265920 cpu: 1.3

(Enter /home/kira/g09/l401.exe)

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

B after Tr= -0.000000 0.000000 0.000000

Rot= 1.000000 -0.000000 0.000000 0.000033 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

Occupied (A') (A') (A") (A') (A') (A") (A') (A") (A") (A')

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The electronic state of the initial guess is 2-A'.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7585 S= 0.5043

Generating alternative initial guess.

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2000

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= -1914.58024534267

Leave Link 401 at Sun Aug 18 14:10:35 2019, MaxMem= 2013265920 cpu: 49.3

(Enter /home/kira/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3047318 IEndB= 3047318 NGot= 2013265920 MDV= 2011240249

LenX= 2011240249 LenY= 2010235243

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= 480000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 97949388.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.77D-15 for 5713.

Iteration 1 A\*A^-1 deviation from orthogonality is 5.11D-15 for 5691 4661.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.77D-15 for 5673.

Iteration 1 A^-1\*A deviation from orthogonality is 4.36D-09 for 3254 3236.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.44D-15 for 777.

Iteration 2 A\*A^-1 deviation from orthogonality is 3.55D-15 for 5499 161.

Iteration 2 A^-1\*A deviation from unit magnitude is 8.88D-16 for 1068.

Iteration 2 A^-1\*A deviation from orthogonality is 4.35D-16 for 2462 2427.

E= -1914.35956816695

DIIS: error= 1.26D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.35956816695 IErMin= 1 ErrMin= 1.26D-02

ErrMax= 1.26D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.46D-01 BMatP= 2.46D-01

IDIUse=3 WtCom= 8.74D-01 WtEn= 1.26D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Recover alternate guess density for next cycle.

RMSDP=1.17D-03 MaxDP=5.84D-02 OVMax= 0.00D+00

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.17D-03 CP: 9.91D-01

E= -1913.46850744426 Delta-E= 0.891060722688 Rises=F Damp=F

Switch densities from cycles 1 and 2 for lowest energy.

DIIS: error= 4.61D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 1 EnMin= -1914.35956816695 IErMin= 1 ErrMin= 1.26D-02

ErrMax= 4.61D-02 0.00D+00 EMaxC= 1.00D+00 BMatC= 4.26D+00 BMatP= 2.46D-01

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

Coeff-Com: 0.944D+00 0.556D-01

Coeff: 0.944D+00 0.556D-01

Gap= 0.445 Goal= None Shift= 0.000

Gap= 0.503 Goal= None Shift= 0.000

RMSDP=5.39D-03 MaxDP=3.32D-01 DE= 8.91D-01 OVMax= 6.38D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.50D-04 CP: 9.98D-01 6.07D-02

E= -1914.48866213029 Delta-E= -1.020154686027 Rises=F Damp=F

DIIS: error= 1.95D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.48866213029 IErMin= 3 ErrMin= 1.95D-03

ErrMax= 1.95D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.33D-02 BMatP= 2.46D-01

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

Coeff-Com: -0.541D-01 0.441D-01 0.101D+01

Coeff: -0.541D-01 0.441D-01 0.101D+01

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=9.34D-05 MaxDP=4.43D-03 DE=-1.02D+00 OVMax= 1.24D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 7.26D-05 CP: 9.98D-01 1.11D-01 1.01D+00

E= -1914.49261482468 Delta-E= -0.003952694385 Rises=F Damp=F

DIIS: error= 8.06D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.49261482468 IErMin= 4 ErrMin= 8.06D-04

ErrMax= 8.06D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.70D-03 BMatP= 1.33D-02

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

Coeff-Com: -0.308D-01 0.121D-01 0.415D+00 0.603D+00

Coeff: -0.308D-01 0.121D-01 0.415D+00 0.603D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=3.72D-05 MaxDP=1.90D-03 DE=-3.95D-03 OVMax= 8.81D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.90D-05 CP: 9.98D-01 1.07D-01 1.04D+00 7.06D-01

E= -1914.49316078063 Delta-E= -0.000545955955 Rises=F Damp=F

DIIS: error= 3.50D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.49316078063 IErMin= 5 ErrMin= 3.50D-04

ErrMax= 3.50D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 5.42D-04 BMatP= 2.70D-03

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

Coeff-Com: -0.971D-02 0.112D-02 0.101D+00 0.341D+00 0.567D+00

Coeff: -0.971D-02 0.112D-02 0.101D+00 0.341D+00 0.567D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=1.56D-05 MaxDP=8.66D-04 DE=-5.46D-04 OVMax= 3.03D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 9.27D-06 CP: 9.98D-01 1.07D-01 1.04D+00 7.66D-01 5.99D-01

E= -1914.49330207325 Delta-E= -0.000141292617 Rises=F Damp=F

DIIS: error= 1.06D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.49330207325 IErMin= 6 ErrMin= 1.06D-04

ErrMax= 1.06D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.42D-05 BMatP= 5.42D-04

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

Coeff-Com: -0.196D-02-0.388D-03 0.107D-01 0.960D-01 0.241D+00 0.655D+00

Coeff: -0.196D-02-0.388D-03 0.107D-01 0.960D-01 0.241D+00 0.655D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=4.89D-06 MaxDP=2.28D-04 DE=-1.41D-04 OVMax= 8.33D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 3.04D-06 CP: 9.98D-01 1.07D-01 1.04D+00 7.86D-01 6.58D-01

CP: 6.89D-01

E= -1914.49330639779 Delta-E= -0.000004324543 Rises=F Damp=F

DIIS: error= 6.39D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.49330639779 IErMin= 7 ErrMin= 6.39D-05

ErrMax= 6.39D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 8.62D-06 BMatP= 2.42D-05

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

Coeff-Com: 0.232D-04-0.362D-03-0.693D-02 0.142D-01 0.755D-01 0.413D+00

Coeff-Com: 0.505D+00

Coeff: 0.232D-04-0.362D-03-0.693D-02 0.142D-01 0.755D-01 0.413D+00

Coeff: 0.505D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=1.94D-06 MaxDP=1.19D-04 DE=-4.32D-06 OVMax= 4.89D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 8.08D-07 CP: 9.98D-01 1.07D-01 1.04D+00 7.86D-01 6.61D-01

CP: 7.94D-01 5.51D-01

E= -1914.49330849040 Delta-E= -0.000002092608 Rises=F Damp=F

DIIS: error= 1.52D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.49330849040 IErMin= 8 ErrMin= 1.52D-05

ErrMax= 1.52D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.95D-07 BMatP= 8.62D-06

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

Coeff-Com: 0.175D-03-0.136D-03-0.431D-02-0.153D-02 0.150D-01 0.139D+00

Coeff-Com: 0.240D+00 0.611D+00

Coeff: 0.175D-03-0.136D-03-0.431D-02-0.153D-02 0.150D-01 0.139D+00

Coeff: 0.240D+00 0.611D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=4.98D-07 MaxDP=3.32D-05 DE=-2.09D-06 OVMax= 1.45D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 3.88D-07 CP: 9.98D-01 1.07D-01 1.04D+00 7.87D-01 6.64D-01

CP: 7.86D-01 5.98D-01 7.20D-01

E= -1914.49330857630 Delta-E= -0.000000085900 Rises=F Damp=F

DIIS: error= 7.40D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.49330857630 IErMin= 9 ErrMin= 7.40D-06

ErrMax= 7.40D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 8.64D-08 BMatP= 3.95D-07

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

Coeff-Com: 0.913D-04-0.127D-04-0.138D-02-0.297D-02-0.313D-02 0.169D-01

Coeff-Com: 0.622D-01 0.350D+00 0.578D+00

Coeff: 0.913D-04-0.127D-04-0.138D-02-0.297D-02-0.313D-02 0.169D-01

Coeff: 0.622D-01 0.350D+00 0.578D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=2.04D-07 MaxDP=1.41D-05 DE=-8.59D-08 OVMax= 5.48D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.26D-07 CP: 9.98D-01 1.07D-01 1.04D+00 7.87D-01 6.64D-01

CP: 7.94D-01 5.95D-01 8.50D-01 7.98D-01

E= -1914.49330860037 Delta-E= -0.000000024072 Rises=F Damp=F

DIIS: error= 3.32D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.49330860037 IErMin=10 ErrMin= 3.32D-06

ErrMax= 3.32D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 7.00D-09 BMatP= 8.64D-08

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

Coeff-Com: 0.121D-04 0.121D-04 0.112D-04-0.844D-03-0.298D-02-0.962D-02

Coeff-Com: -0.504D-02 0.523D-01 0.202D+00 0.764D+00

Coeff: 0.121D-04 0.121D-04 0.112D-04-0.844D-03-0.298D-02-0.962D-02

Coeff: -0.504D-02 0.523D-01 0.202D+00 0.764D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=8.58D-08 MaxDP=6.72D-06 DE=-2.41D-08 OVMax= 2.52D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 6.53D-08 CP: 9.98D-01 1.07D-01 1.04D+00 7.87D-01 6.64D-01

CP: 7.93D-01 6.04D-01 8.79D-01 8.92D-01 1.05D+00

E= -1914.49330860521 Delta-E= -0.000000004837 Rises=F Damp=F

DIIS: error= 2.48D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.49330860521 IErMin=11 ErrMin= 2.48D-06

ErrMax= 2.48D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.19D-09 BMatP= 7.00D-09

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

Coeff-Com: -0.286D-04 0.103D-04 0.557D-03 0.702D-03-0.506D-03-0.119D-01

Coeff-Com: -0.270D-01-0.110D+00-0.117D+00 0.423D+00 0.843D+00

Coeff: -0.286D-04 0.103D-04 0.557D-03 0.702D-03-0.506D-03-0.119D-01

Coeff: -0.270D-01-0.110D+00-0.117D+00 0.423D+00 0.843D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=7.04D-08 MaxDP=5.32D-06 DE=-4.84D-09 OVMax= 2.26D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 3.73D-08 CP: 9.98D-01 1.07D-01 1.04D+00 7.87D-01 6.64D-01

CP: 7.94D-01 6.04D-01 9.03D-01 9.64D-01 1.41D+00

CP: 1.25D+00

E= -1914.49330860808 Delta-E= -0.000000002869 Rises=F Damp=F

DIIS: error= 1.17D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.49330860808 IErMin=12 ErrMin= 1.17D-06

ErrMax= 1.17D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 6.61D-10 BMatP= 3.19D-09

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

Coeff-Com: -0.139D-04-0.771D-06 0.202D-03 0.540D-03 0.751D-03-0.160D-02

Coeff-Com: -0.892D-02-0.570D-01-0.100D+00-0.459D-01 0.317D+00 0.895D+00

Coeff: -0.139D-04-0.771D-06 0.202D-03 0.540D-03 0.751D-03-0.160D-02

Coeff: -0.892D-02-0.570D-01-0.100D+00-0.459D-01 0.317D+00 0.895D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=4.04D-08 MaxDP=2.40D-06 DE=-2.87D-09 OVMax= 1.31D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.91D-08 CP: 9.98D-01 1.07D-01 1.04D+00 7.87D-01 6.64D-01

CP: 7.95D-01 6.05D-01 9.12D-01 1.00D+00 1.57D+00

CP: 1.59D+00 1.18D+00

E= -1914.49330860894 Delta-E= -0.000000000866 Rises=F Damp=F

DIIS: error= 5.59D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1914.49330860894 IErMin=13 ErrMin= 5.59D-07

ErrMax= 5.59D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.99D-10 BMatP= 6.61D-10

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

Coeff-Com: -0.108D-05-0.286D-05-0.259D-04 0.137D-03 0.581D-03 0.210D-02

Coeff-Com: 0.163D-02-0.508D-02-0.289D-01-0.137D+00-0.356D-01 0.530D+00

Coeff-Com: 0.672D+00

Coeff: -0.108D-05-0.286D-05-0.259D-04 0.137D-03 0.581D-03 0.210D-02

Coeff: 0.163D-02-0.508D-02-0.289D-01-0.137D+00-0.356D-01 0.530D+00

Coeff: 0.672D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=1.93D-08 MaxDP=7.91D-07 DE=-8.66D-10 OVMax= 5.93D-06

Cycle 14 Pass 1 IDiag 1:

RMSU= 9.91D-09 CP: 9.98D-01 1.07D-01 1.04D+00 7.87D-01 6.64D-01

CP: 7.95D-01 6.05D-01 9.15D-01 1.01D+00 1.64D+00

CP: 1.73D+00 1.44D+00 1.00D+00

E= -1914.49330860923 Delta-E= -0.000000000288 Rises=F Damp=F

DIIS: error= 1.98D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1914.49330860923 IErMin=14 ErrMin= 1.98D-07

ErrMax= 1.98D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 5.77D-11 BMatP= 2.99D-10

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

Coeff-Com: 0.334D-05-0.550D-06-0.665D-04-0.956D-04 0.243D-04 0.127D-02

Coeff-Com: 0.320D-02 0.142D-01 0.171D-01-0.446D-01-0.107D+00-0.263D-01

Coeff-Com: 0.289D+00 0.854D+00

Coeff: 0.334D-05-0.550D-06-0.665D-04-0.956D-04 0.243D-04 0.127D-02

Coeff: 0.320D-02 0.142D-01 0.171D-01-0.446D-01-0.107D+00-0.263D-01

Coeff: 0.289D+00 0.854D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=1.05D-08 MaxDP=5.23D-07 DE=-2.88D-10 OVMax= 3.29D-06

Cycle 15 Pass 1 IDiag 1:

RMSU= 4.78D-09 CP: 9.98D-01 1.07D-01 1.04D+00 7.87D-01 6.64D-01

CP: 7.95D-01 6.05D-01 9.17D-01 1.01D+00 1.66D+00

CP: 1.81D+00 1.56D+00 1.29D+00 1.10D+00

E= -1914.49330860926 Delta-E= -0.000000000033 Rises=F Damp=F

DIIS: error= 1.21D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1914.49330860926 IErMin=15 ErrMin= 1.21D-07

ErrMax= 1.21D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.39D-11 BMatP= 5.77D-11

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

Coeff-Com: 0.235D-05 0.513D-06-0.327D-04-0.101D-03-0.165D-03 0.155D-03

Coeff-Com: 0.149D-02 0.100D-01 0.190D-01 0.140D-01-0.530D-01-0.176D+00

Coeff-Com: -0.311D-01 0.515D+00 0.700D+00

Coeff: 0.235D-05 0.513D-06-0.327D-04-0.101D-03-0.165D-03 0.155D-03

Coeff: 0.149D-02 0.100D-01 0.190D-01 0.140D-01-0.530D-01-0.176D+00

Coeff: -0.311D-01 0.515D+00 0.700D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=5.35D-09 MaxDP=2.95D-07 DE=-3.27D-11 OVMax= 1.67D-06

Error on total polarization charges = 0.08609

SCF Done: E(UB3LYP) = -1914.49330861 A.U. after 15 cycles

NFock= 15 Conv=0.54D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7585 S= 0.5042

<L.S>= 0.000000000000E+00

KE= 1.906555955226D+03 PE=-1.517667338024D+04 EE= 6.009767223676D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.25

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7585, after 0.7500

Leave Link 502 at Sun Aug 18 14:19:41 2019, MaxMem= 2013265920 cpu: 4343.2

(Enter /home/kira/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 = 183

Leave Link 701 at Sun Aug 18 14:19:58 2019, MaxMem= 2013265920 cpu: 136.9

(Enter /home/kira/g09/l702.exe)

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

Leave Link 702 at Sun Aug 18 14:19:58 2019, MaxMem= 2013265920 cpu: 0.2

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 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= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

Petite list used in FoFCou.

Leave Link 703 at Sun Aug 18 14:21:13 2019, MaxMem= 2013265920 cpu: 600.6

(Enter /home/kira/g09/l716.exe)

Dipole = 4.84817762D-04-1.86138941D-01-5.42677014D-13

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.001777281 -0.000381540 0.003423491

2 6 0.002519730 0.000581222 -0.006243157

3 7 0.002288442 -0.000977660 0.000000000

4 6 0.002519730 0.000581222 0.006243157

5 6 -0.001777281 -0.000381540 -0.003423491

6 6 -0.001409911 -0.000425675 -0.002656935

7 6 -0.000055576 0.000590788 -0.002097876

8 7 0.000003390 -0.000419270 -0.000371727

9 6 0.000103512 0.000644127 -0.002136972

10 6 -0.001444082 -0.000271434 0.001072425

11 6 0.001426879 -0.000254046 0.001078811

12 6 -0.001409911 -0.000425675 0.002656935

13 6 -0.000055576 0.000590788 0.002097876

14 6 0.001426879 -0.000254046 -0.001078811

15 6 -0.001444082 -0.000271434 -0.001072425

16 6 0.000103512 0.000644127 0.002136972

17 7 0.000003390 -0.000419270 0.000371727

18 6 0.001339370 -0.000348136 0.002571035

19 6 -0.002517131 0.000461376 -0.006179976

20 6 0.001824602 -0.000411357 0.003471366

21 6 0.001824602 -0.000411357 -0.003471366

22 6 -0.002517131 0.000461376 0.006179975

23 7 -0.002220486 -0.000662151 -0.000000000

24 6 0.001339370 -0.000348136 -0.002571035

25 6 0.001138100 0.000348303 -0.000983951

26 6 -0.000734891 0.000690199 0.001011490

27 6 0.000178667 -0.000220034 -0.000426883

28 6 -0.000256261 0.000058389 0.000356750

29 6 0.000471132 0.000147169 -0.000302307

30 6 -0.001106613 -0.000674769 0.000711778

31 6 -0.000256261 0.000058389 -0.000356750

32 6 0.000178667 -0.000220034 0.000426883

33 6 -0.000734891 0.000690199 -0.001011490

34 6 0.001138100 0.000348303 0.000983951

35 6 -0.001106613 -0.000674769 -0.000711778

36 6 0.000471132 0.000147169 0.000302307

37 6 -0.001133257 0.000317965 -0.001041678

38 6 0.001109883 -0.000676153 0.000750856

39 6 -0.000493922 0.000139458 -0.000300139

40 6 0.000270734 0.000037241 0.000356282

41 6 -0.000166073 -0.000199513 -0.000436702

42 6 0.000764520 0.000695809 0.001015605

43 6 -0.001133257 0.000317965 0.001041678

44 6 0.001109883 -0.000676153 -0.000750856

45 6 -0.000493922 0.000139458 0.000300139

46 6 0.000270734 0.000037241 -0.000356282

47 6 -0.000166073 -0.000199513 0.000436702

48 6 0.000764520 0.000695809 -0.001015605

49 1 -0.000195852 0.000155077 0.000171724

50 1 -0.000195852 0.000155077 -0.000171725

51 1 -0.000040894 -0.000145204 0.000167611

52 1 0.000033588 -0.000135816 0.000171658

53 1 0.000033588 -0.000135816 -0.000171658

54 1 -0.000040894 -0.000145204 -0.000167611

55 1 0.000184660 0.000167232 0.000175820

56 1 0.000184660 0.000167232 -0.000175820

57 1 0.000089096 -0.000241385 0.000085954

58 1 -0.000067075 -0.000082959 -0.000092729

59 1 0.000005062 -0.000005671 -0.000002322

60 1 0.000112540 0.000072327 0.000049316

61 1 0.000016141 0.000249375 -0.000040222

62 1 0.000005062 -0.000005671 0.000002322

63 1 -0.000067075 -0.000082959 0.000092729

64 1 0.000089096 -0.000241385 -0.000085954

65 1 0.000016141 0.000249375 0.000040222

66 1 0.000112540 0.000072327 -0.000049315

67 1 -0.000024599 0.000237782 -0.000028431

68 1 -0.000115832 0.000068722 0.000053959

69 1 -0.000004765 -0.000007036 -0.000004030

70 1 0.000070622 -0.000081467 -0.000096839

71 1 -0.000091398 -0.000246714 0.000096552

72 1 -0.000024599 0.000237782 0.000028431

73 1 -0.000115832 0.000068722 -0.000053959

74 1 -0.000004765 -0.000007036 0.000004030

75 1 0.000070622 -0.000081467 0.000096839

76 1 -0.000091398 -0.000246714 -0.000096552

77 1 0.000145281 0.000391528 0.000000000

78 1 -0.000266864 0.000379517 -0.000000000

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

Cartesian Forces: Max 0.006243157 RMS 0.001230049

Leave Link 716 at Sun Aug 18 14:21:13 2019, MaxMem= 2013265920 cpu: 0.2

(Enter /home/kira/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 0.003718995 RMS 0.000582728

Search for a local minimum.

Step number 4 out of a maximum of 452

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

RMS Force = .58273D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 2 3 4

DE= -4.14D-04 DEPred=-4.36D-04 R= 9.48D-01

TightC=F SS= 1.41D+00 RLast= 4.28D-01 DXNew= 9.5899D-01 1.2852D+00

Trust test= 9.48D-01 RLast= 4.28D-01 DXMaxT set to 9.59D-01

ITU= 1 1 1 0

Eigenvalues --- 0.00509 0.00983 0.00987 0.00988 0.01472

Eigenvalues --- 0.01615 0.01619 0.01626 0.01638 0.01659

Eigenvalues --- 0.01721 0.01721 0.01721 0.01724 0.01738

Eigenvalues --- 0.01752 0.01758 0.01775 0.01787 0.01792

Eigenvalues --- 0.01837 0.01848 0.01855 0.01891 0.01901

Eigenvalues --- 0.01923 0.01932 0.01943 0.01988 0.01992

Eigenvalues --- 0.02010 0.02020 0.02023 0.02027 0.02068

Eigenvalues --- 0.02068 0.02070 0.02070 0.02077 0.02081

Eigenvalues --- 0.02104 0.02106 0.02118 0.02119 0.02119

Eigenvalues --- 0.02130 0.02130 0.02131 0.02132 0.02132

Eigenvalues --- 0.02132 0.02158 0.02160 0.02160 0.02160

Eigenvalues --- 0.02162 0.02162 0.02162 0.02164 0.02173

Eigenvalues --- 0.02173 0.02173 0.02174 0.02181 0.02181

Eigenvalues --- 0.02181 0.02184 0.02186 0.02187 0.02187

Eigenvalues --- 0.02189 0.02216 0.02216 0.02238 0.02808

Eigenvalues --- 0.15861 0.15890 0.15994 0.15995 0.15995

Eigenvalues --- 0.15995 0.15995 0.15997 0.15997 0.15998

Eigenvalues --- 0.15999 0.15999 0.15999 0.15999 0.15999

Eigenvalues --- 0.15999 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16003 0.16127

Eigenvalues --- 0.22000 0.22000 0.22000 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22004 0.22753 0.22768

Eigenvalues --- 0.22814 0.22829 0.23470 0.23470 0.23470

Eigenvalues --- 0.23540 0.23586 0.24263 0.24728 0.24815

Eigenvalues --- 0.24876 0.24889 0.24979 0.24995 0.24999

Eigenvalues --- 0.24999 0.24999 0.24999 0.24999 0.24999

Eigenvalues --- 0.24999 0.25000 0.25000 0.25000 0.25036

Eigenvalues --- 0.26341 0.28232 0.34159 0.34182 0.34206

Eigenvalues --- 0.34823 0.35413 0.35413 0.35413 0.35414

Eigenvalues --- 0.35415 0.35415 0.35416 0.35416 0.35416

Eigenvalues --- 0.35416 0.35416 0.35455 0.35506 0.35507

Eigenvalues --- 0.35508 0.35523 0.35542 0.35544 0.35547

Eigenvalues --- 0.35642 0.36056 0.36057 0.36058 0.36113

Eigenvalues --- 0.36250 0.36250 0.36251 0.36276 0.37129

Eigenvalues --- 0.37169 0.37254 0.37290 0.39127 0.39396

Eigenvalues --- 0.39745 0.40113 0.40260 0.40420 0.40463

Eigenvalues --- 0.41184 0.41795 0.41802 0.41810 0.42028

Eigenvalues --- 0.42075 0.42077 0.42079 0.42085 0.43286

Eigenvalues --- 0.44668 0.45044 0.45324 0.45570 0.45571

Eigenvalues --- 0.45586 0.45587 0.45702 0.45769 0.45844

Eigenvalues --- 0.45873 0.45930 0.45937 0.45942 0.45948

Eigenvalues --- 0.45970 0.46660 0.46661 0.46661 0.46667

Eigenvalues --- 0.47073 0.47079 0.47086 0.47450 0.48193

Eigenvalues --- 0.48279 0.49332 0.49431 0.49974 0.50485

Eigenvalues --- 0.50810 0.53956 0.63934

En-DIIS/RFO-DIIS IScMMF= 0 using points: 4 3 2

RFO step: Lambda=-2.06574272D-04.

NNeg= 0 NP= 3 Switch= 2.50D-03 Rises=F DC= 4.14D-04 SmlDif= 1.00D-05

RMS Error= 0.9031414347D-03 NUsed= 3 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 0.66238 0.15662 0.18100

Iteration 1 RMS(Cart)= 0.02976629 RMS(Int)= 0.00024133

Iteration 2 RMS(Cart)= 0.00041202 RMS(Int)= 0.00010362

Iteration 3 RMS(Cart)= 0.00000007 RMS(Int)= 0.00010362

ITry= 1 IFail=0 DXMaxC= 1.08D-01 DCOld= 1.00D+10 DXMaxT= 9.59D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 2.03D-08 for atom 62.

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

(Linear) (Quad) (Total)

R1 2.73469 -0.00225 -0.00355 -0.00119 -0.00479 2.72991

R2 2.56644 0.00233 0.00379 0.00097 0.00462 2.57106

R3 2.03873 -0.00007 -0.00021 0.00005 -0.00017 2.03856

R4 2.62451 -0.00205 -0.00228 -0.00156 -0.00373 2.62078

R5 2.60891 0.00372 0.00468 0.00207 0.00675 2.61566

R6 2.62451 -0.00205 -0.00228 -0.00156 -0.00373 2.62078

R7 1.91028 -0.00014 -0.00037 0.00005 -0.00032 1.90996

R8 2.73469 -0.00225 -0.00355 -0.00119 -0.00479 2.72991

R9 2.60891 0.00372 0.00468 0.00207 0.00675 2.61566

R10 2.03873 -0.00007 -0.00021 0.00005 -0.00017 2.03856

R11 2.70362 0.00050 0.00077 0.00005 0.00081 2.70444

R12 2.82083 -0.00038 -0.00154 0.00006 -0.00148 2.81935

R13 2.59272 -0.00006 0.00058 -0.00057 0.00014 2.59286

R14 2.71947 -0.00120 -0.00173 -0.00075 -0.00252 2.71695

R15 2.59280 -0.00006 0.00056 -0.00055 0.00013 2.59293

R16 2.71966 -0.00122 -0.00182 -0.00073 -0.00259 2.71707

R17 2.70356 0.00053 0.00089 0.00003 0.00092 2.70448

R18 2.59660 0.00156 0.00186 0.00089 0.00259 2.59919

R19 2.04125 -0.00012 0.00004 -0.00016 -0.00012 2.04114

R20 2.04131 -0.00013 0.00001 -0.00015 -0.00014 2.04117

R21 2.70362 0.00050 0.00077 0.00005 0.00081 2.70444

R22 2.82083 -0.00038 -0.00154 0.00006 -0.00148 2.81935

R23 2.71947 -0.00120 -0.00173 -0.00075 -0.00252 2.71695

R24 2.59272 -0.00006 0.00058 -0.00057 0.00014 2.59286

R25 2.59660 0.00156 0.00186 0.00089 0.00259 2.59919

R26 2.04131 -0.00013 0.00001 -0.00015 -0.00014 2.04117

R27 2.71966 -0.00122 -0.00182 -0.00073 -0.00259 2.71707

R28 2.04125 -0.00012 0.00004 -0.00016 -0.00012 2.04114

R29 2.59280 -0.00006 0.00056 -0.00055 0.00013 2.59293

R30 2.70356 0.00053 0.00089 0.00003 0.00092 2.70448

R31 2.60932 0.00366 0.00466 0.00202 0.00669 2.61601

R32 2.82081 -0.00040 -0.00173 0.00013 -0.00160 2.81921

R33 2.73480 -0.00228 -0.00362 -0.00120 -0.00487 2.72993

R34 2.62439 -0.00205 -0.00232 -0.00153 -0.00373 2.62066

R35 2.56633 0.00237 0.00384 0.00100 0.00469 2.57102

R36 2.03867 -0.00006 -0.00019 0.00005 -0.00014 2.03853

R37 2.73480 -0.00228 -0.00362 -0.00120 -0.00487 2.72993

R38 2.03867 -0.00006 -0.00019 0.00005 -0.00014 2.03853

R39 2.62439 -0.00205 -0.00232 -0.00153 -0.00373 2.62066

R40 2.60932 0.00366 0.00466 0.00202 0.00669 2.61601

R41 1.91050 -0.00026 -0.00056 -0.00000 -0.00056 1.90994

R42 2.82081 -0.00040 -0.00173 0.00013 -0.00160 2.81921

R43 2.64748 -0.00038 0.00087 -0.00101 -0.00014 2.64735

R44 2.64931 -0.00024 0.00082 -0.00079 0.00004 2.64935

R45 2.63348 0.00024 0.00014 0.00020 0.00034 2.63382

R46 2.05056 -0.00014 -0.00049 0.00005 -0.00044 2.05013

R47 2.63424 -0.00016 -0.00020 -0.00010 -0.00030 2.63394

R48 2.05112 -0.00010 -0.00002 -0.00015 -0.00017 2.05095

R49 2.63678 -0.00010 -0.00014 -0.00004 -0.00018 2.63660

R50 2.05040 0.00001 0.00007 -0.00003 0.00004 2.05043

R51 2.63015 0.00037 0.00023 0.00034 0.00057 2.63073

R52 2.05110 -0.00008 -0.00000 -0.00014 -0.00014 2.05095

R53 2.05040 -0.00020 -0.00054 -0.00001 -0.00055 2.04985

R54 2.63424 -0.00016 -0.00020 -0.00010 -0.00030 2.63394

R55 2.63678 -0.00010 -0.00014 -0.00004 -0.00018 2.63660

R56 2.05040 0.00001 0.00007 -0.00003 0.00004 2.05043

R57 2.63348 0.00024 0.00014 0.00020 0.00034 2.63382

R58 2.05112 -0.00010 -0.00002 -0.00015 -0.00017 2.05095

R59 2.64748 -0.00038 0.00087 -0.00101 -0.00014 2.64735

R60 2.05056 -0.00014 -0.00049 0.00005 -0.00044 2.05013

R61 2.64931 -0.00024 0.00082 -0.00079 0.00004 2.64935

R62 2.63015 0.00037 0.00023 0.00034 0.00057 2.63073

R63 2.05040 -0.00020 -0.00054 -0.00001 -0.00055 2.04985

R64 2.05110 -0.00008 -0.00000 -0.00014 -0.00014 2.05095

R65 2.64944 -0.00026 0.00088 -0.00084 0.00004 2.64948

R66 2.64762 -0.00041 0.00090 -0.00105 -0.00015 2.64746

R67 2.63013 0.00036 0.00020 0.00035 0.00056 2.63068

R68 2.05037 -0.00020 -0.00056 0.00001 -0.00055 2.04982

R69 2.63679 -0.00012 -0.00013 -0.00007 -0.00019 2.63660

R70 2.05110 -0.00008 -0.00000 -0.00014 -0.00014 2.05096

R71 2.63420 -0.00014 -0.00020 -0.00007 -0.00027 2.63393

R72 2.05039 0.00001 0.00007 -0.00003 0.00004 2.05043

R73 2.63343 0.00025 0.00015 0.00021 0.00035 2.63378

R74 2.05113 -0.00010 -0.00003 -0.00015 -0.00018 2.05095

R75 2.05053 -0.00014 -0.00048 0.00005 -0.00043 2.05010

R76 2.64944 -0.00026 0.00088 -0.00084 0.00004 2.64948

R77 2.64762 -0.00041 0.00090 -0.00105 -0.00015 2.64746

R78 2.63013 0.00036 0.00020 0.00035 0.00056 2.63068

R79 2.05037 -0.00020 -0.00056 0.00001 -0.00055 2.04982

R80 2.63679 -0.00012 -0.00013 -0.00007 -0.00019 2.63660

R81 2.05110 -0.00008 -0.00000 -0.00014 -0.00014 2.05096

R82 2.63420 -0.00014 -0.00020 -0.00007 -0.00027 2.63393

R83 2.05039 0.00001 0.00007 -0.00003 0.00004 2.05043

R84 2.63343 0.00025 0.00015 0.00021 0.00035 2.63378

R85 2.05113 -0.00010 -0.00003 -0.00015 -0.00018 2.05095

R86 2.05053 -0.00014 -0.00048 0.00005 -0.00043 2.05010

A1 1.89856 -0.00068 -0.00085 -0.00055 -0.00135 1.89722

A2 2.17360 0.00007 0.00038 -0.00068 -0.00034 2.17326

A3 2.21088 0.00061 0.00046 0.00131 0.00174 2.21261

A4 1.84471 0.00044 0.00047 0.00058 0.00110 1.84581

A5 2.22108 -0.00039 0.00023 -0.00053 -0.00070 2.22039

A6 2.21737 -0.00005 -0.00070 -0.00007 -0.00041 2.21696

A7 1.93822 0.00049 0.00058 -0.00006 0.00049 1.93870

A8 2.16968 -0.00023 0.00026 0.00011 0.00046 2.17014

A9 2.16968 -0.00023 0.00026 0.00011 0.00046 2.17014

A10 1.84471 0.00044 0.00047 0.00058 0.00110 1.84581

A11 2.21737 -0.00005 -0.00070 -0.00007 -0.00041 2.21696

A12 2.22108 -0.00039 0.00023 -0.00053 -0.00070 2.22039

A13 1.89856 -0.00068 -0.00085 -0.00055 -0.00135 1.89722

A14 2.21088 0.00061 0.00046 0.00131 0.00174 2.21261

A15 2.17360 0.00007 0.00038 -0.00068 -0.00034 2.17326

A16 2.18844 0.00107 -0.00131 0.00275 0.00196 2.19040

A17 2.04775 -0.00084 0.00008 -0.00165 -0.00182 2.04593

A18 2.04693 -0.00023 0.00125 -0.00108 -0.00009 2.04685

A19 2.19609 -0.00049 -0.00192 -0.00066 -0.00218 2.19390

A20 2.15679 0.00079 0.00229 0.00086 0.00275 2.15954

A21 1.93029 -0.00030 -0.00041 -0.00019 -0.00056 1.92973

A22 1.84782 0.00060 0.00042 0.00073 0.00101 1.84883

A23 1.93013 -0.00028 -0.00037 -0.00016 -0.00051 1.92963

A24 2.19595 -0.00049 -0.00183 -0.00070 -0.00211 2.19384

A25 2.15709 0.00077 0.00216 0.00087 0.00263 2.15971

A26 1.85814 -0.00001 0.00014 -0.00006 0.00011 1.85825

A27 2.20402 -0.00014 -0.00028 -0.00043 -0.00073 2.20329

A28 2.22089 0.00015 0.00014 0.00050 0.00063 2.22151

A29 1.85806 0.00000 0.00013 -0.00002 0.00014 1.85820

A30 2.20391 -0.00014 -0.00018 -0.00048 -0.00067 2.20324

A31 2.22107 0.00014 0.00006 0.00051 0.00056 2.22163

A32 2.18844 0.00107 -0.00131 0.00275 0.00196 2.19040

A33 2.04775 -0.00084 0.00008 -0.00165 -0.00182 2.04593

A34 2.04693 -0.00023 0.00125 -0.00108 -0.00009 2.04685

A35 2.15679 0.00079 0.00229 0.00086 0.00275 2.15954

A36 2.19609 -0.00049 -0.00192 -0.00066 -0.00218 2.19390

A37 1.93029 -0.00030 -0.00041 -0.00019 -0.00056 1.92973

A38 1.85806 0.00000 0.00013 -0.00002 0.00014 1.85820

A39 2.20391 -0.00014 -0.00018 -0.00048 -0.00067 2.20324

A40 2.22107 0.00014 0.00006 0.00051 0.00056 2.22163

A41 1.85814 -0.00001 0.00014 -0.00006 0.00011 1.85825

A42 2.22089 0.00015 0.00014 0.00050 0.00063 2.22151

A43 2.20402 -0.00014 -0.00028 -0.00043 -0.00073 2.20329

A44 1.93013 -0.00028 -0.00037 -0.00016 -0.00051 1.92963

A45 2.15709 0.00077 0.00216 0.00087 0.00263 2.15971

A46 2.19595 -0.00049 -0.00183 -0.00070 -0.00211 2.19384

A47 1.84782 0.00060 0.00042 0.00073 0.00101 1.84883

A48 2.18826 0.00109 -0.00136 0.00282 0.00202 2.19028

A49 2.04725 -0.00028 0.00138 -0.00130 -0.00020 2.04704

A50 2.04763 -0.00081 -0.00000 -0.00151 -0.00179 2.04584

A51 2.22105 -0.00037 0.00027 -0.00050 -0.00067 2.22038

A52 2.21751 -0.00006 -0.00069 -0.00011 -0.00039 2.21712

A53 1.84460 0.00043 0.00043 0.00059 0.00105 1.84566

A54 1.89858 -0.00068 -0.00085 -0.00055 -0.00133 1.89725

A55 2.17371 0.00008 0.00029 -0.00063 -0.00037 2.17334

A56 2.21074 0.00061 0.00053 0.00124 0.00174 2.21248

A57 1.89858 -0.00068 -0.00085 -0.00055 -0.00133 1.89725

A58 2.21074 0.00061 0.00053 0.00124 0.00174 2.21248

A59 2.17371 0.00008 0.00029 -0.00063 -0.00037 2.17334

A60 1.84460 0.00043 0.00043 0.00059 0.00105 1.84566

A61 2.22105 -0.00037 0.00027 -0.00050 -0.00067 2.22038

A62 2.21751 -0.00006 -0.00069 -0.00011 -0.00039 2.21712

A63 1.93840 0.00051 0.00064 -0.00008 0.00054 1.93894

A64 2.17017 -0.00024 0.00019 -0.00007 0.00026 2.17043

A65 2.17017 -0.00024 0.00019 -0.00007 0.00026 2.17043

A66 2.18826 0.00109 -0.00136 0.00282 0.00202 2.19028

A67 2.04725 -0.00028 0.00138 -0.00130 -0.00020 2.04704

A68 2.04763 -0.00081 -0.00000 -0.00151 -0.00179 2.04584

A69 2.11769 -0.00068 -0.00040 -0.00151 -0.00191 2.11578

A70 2.10414 -0.00034 0.00035 -0.00107 -0.00071 2.10342

A71 2.06136 0.00102 0.00005 0.00257 0.00262 2.06398

A72 2.11233 -0.00060 -0.00029 -0.00145 -0.00174 2.11060

A73 2.08122 0.00023 -0.00027 0.00068 0.00042 2.08164

A74 2.08958 0.00037 0.00055 0.00079 0.00134 2.09092

A75 2.09775 -0.00002 0.00016 -0.00016 0.00000 2.09775

A76 2.08794 0.00009 0.00043 0.00011 0.00054 2.08848

A77 2.09747 -0.00007 -0.00060 0.00006 -0.00054 2.09694

A78 2.08433 0.00032 0.00024 0.00078 0.00102 2.08534

A79 2.09955 -0.00016 -0.00011 -0.00038 -0.00049 2.09906

A80 2.09931 -0.00017 -0.00013 -0.00040 -0.00053 2.09878

A81 2.09779 -0.00006 0.00017 -0.00021 -0.00005 2.09774

A82 2.09706 -0.00007 -0.00064 0.00006 -0.00058 2.09648

A83 2.08833 0.00013 0.00047 0.00016 0.00063 2.08895

A84 2.11279 -0.00066 -0.00034 -0.00152 -0.00186 2.11093

A85 2.08092 0.00025 -0.00030 0.00068 0.00039 2.08130

A86 2.08945 0.00041 0.00062 0.00085 0.00147 2.09092

A87 2.08433 0.00032 0.00024 0.00078 0.00102 2.08534

A88 2.09955 -0.00016 -0.00011 -0.00038 -0.00049 2.09906

A89 2.09931 -0.00017 -0.00013 -0.00040 -0.00053 2.09878

A90 2.09775 -0.00002 0.00016 -0.00016 0.00000 2.09775

A91 2.09747 -0.00007 -0.00060 0.00006 -0.00054 2.09694

A92 2.08794 0.00009 0.00043 0.00011 0.00054 2.08848

A93 2.11233 -0.00060 -0.00029 -0.00145 -0.00174 2.11060

A94 2.08958 0.00037 0.00055 0.00079 0.00134 2.09092

A95 2.08122 0.00023 -0.00027 0.00068 0.00042 2.08164

A96 2.11769 -0.00068 -0.00040 -0.00151 -0.00191 2.11578

A97 2.10414 -0.00034 0.00035 -0.00107 -0.00071 2.10342

A98 2.06136 0.00102 0.00005 0.00257 0.00262 2.06398

A99 2.11279 -0.00066 -0.00034 -0.00152 -0.00186 2.11093

A100 2.08092 0.00025 -0.00030 0.00068 0.00039 2.08130

A101 2.08945 0.00041 0.00062 0.00085 0.00147 2.09092

A102 2.09779 -0.00006 0.00017 -0.00021 -0.00005 2.09774

A103 2.09706 -0.00007 -0.00064 0.00006 -0.00058 2.09648

A104 2.08833 0.00013 0.00047 0.00016 0.00063 2.08895

A105 2.10444 -0.00039 0.00027 -0.00116 -0.00089 2.10355

A106 2.11766 -0.00065 -0.00031 -0.00148 -0.00179 2.11587

A107 2.06108 0.00104 0.00004 0.00264 0.00268 2.06376

A108 2.11289 -0.00066 -0.00033 -0.00153 -0.00185 2.11103

A109 2.08090 0.00025 -0.00029 0.00068 0.00039 2.08129

A110 2.08936 0.00041 0.00060 0.00086 0.00146 2.09082

A111 2.09787 -0.00007 0.00016 -0.00024 -0.00008 2.09779

A112 2.08826 0.00013 0.00048 0.00017 0.00064 2.08890

A113 2.09705 -0.00006 -0.00064 0.00008 -0.00056 2.09649

A114 2.08422 0.00033 0.00025 0.00079 0.00104 2.08526

A115 2.09937 -0.00017 -0.00014 -0.00042 -0.00055 2.09882

A116 2.09960 -0.00016 -0.00011 -0.00038 -0.00049 2.09911

A117 2.09779 -0.00002 0.00017 -0.00016 0.00001 2.09780

A118 2.09750 -0.00008 -0.00062 0.00006 -0.00056 2.09695

A119 2.08788 0.00010 0.00044 0.00010 0.00055 2.08842

A120 2.11250 -0.00062 -0.00030 -0.00150 -0.00180 2.11070

A121 2.08121 0.00024 -0.00026 0.00069 0.00043 2.08163

A122 2.08943 0.00039 0.00056 0.00083 0.00139 2.09082

A123 2.10444 -0.00039 0.00027 -0.00116 -0.00089 2.10355

A124 2.11766 -0.00065 -0.00031 -0.00148 -0.00179 2.11587

A125 2.06108 0.00104 0.00004 0.00264 0.00268 2.06376

A126 2.11289 -0.00066 -0.00033 -0.00153 -0.00185 2.11103

A127 2.08090 0.00025 -0.00029 0.00068 0.00039 2.08129

A128 2.08936 0.00041 0.00060 0.00086 0.00146 2.09082

A129 2.09787 -0.00007 0.00016 -0.00024 -0.00008 2.09779

A130 2.08826 0.00013 0.00048 0.00017 0.00064 2.08890

A131 2.09705 -0.00006 -0.00064 0.00008 -0.00056 2.09649

A132 2.08422 0.00033 0.00025 0.00079 0.00104 2.08526

A133 2.09937 -0.00017 -0.00014 -0.00042 -0.00055 2.09882

A134 2.09960 -0.00016 -0.00011 -0.00038 -0.00049 2.09911

A135 2.09779 -0.00002 0.00017 -0.00016 0.00001 2.09780

A136 2.09750 -0.00008 -0.00062 0.00006 -0.00056 2.09695

A137 2.08788 0.00010 0.00044 0.00010 0.00055 2.08842

A138 2.11250 -0.00062 -0.00030 -0.00150 -0.00180 2.11070

A139 2.08121 0.00024 -0.00026 0.00069 0.00043 2.08163

A140 2.08943 0.00039 0.00056 0.00083 0.00139 2.09082

D1 -0.00345 0.00013 0.00721 -0.00089 0.00633 0.00289

D2 3.13139 0.00005 0.01114 -0.00491 0.00624 3.13762

D3 -3.12780 -0.00001 0.00790 -0.00498 0.00292 -3.12488

D4 0.00704 -0.00009 0.01183 -0.00901 0.00282 0.00986

D5 0.00000 -0.00000 -0.00000 0.00000 0.00000 0.00000

D6 -3.12388 -0.00013 0.00071 -0.00418 -0.00348 -3.12737

D7 3.12388 0.00013 -0.00071 0.00418 0.00348 3.12737

D8 -0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D9 0.00577 -0.00021 -0.01209 0.00149 -0.01060 -0.00483

D10 3.03773 0.00012 0.00106 0.00310 0.00415 3.04188

D11 -3.12909 -0.00013 -0.01600 0.00551 -0.01050 -3.13959

D12 -0.09712 0.00020 -0.00285 0.00711 0.00425 -0.09287

D13 -3.09241 0.00021 0.01041 -0.00203 0.00838 -3.08403

D14 0.03687 0.00033 0.01474 0.00018 0.01492 0.05179

D15 0.04104 0.00011 0.01514 -0.00688 0.00826 0.04930

D16 -3.11287 0.00023 0.01947 -0.00467 0.01481 -3.09806

D17 -0.00577 0.00021 0.01209 -0.00149 0.01060 0.00483

D18 3.12909 0.00013 0.01600 -0.00551 0.01050 3.13959

D19 -3.03773 -0.00012 -0.00106 -0.00310 -0.00415 -3.04188

D20 0.09712 -0.00020 0.00285 -0.00711 -0.00425 0.09287

D21 0.00345 -0.00013 -0.00721 0.00089 -0.00633 -0.00289

D22 3.12780 0.00001 -0.00790 0.00498 -0.00292 3.12488

D23 -3.13139 -0.00005 -0.01114 0.00491 -0.00624 -3.13762

D24 -0.00704 0.00009 -0.01183 0.00901 -0.00282 -0.00986

D25 -0.04104 -0.00011 -0.01514 0.00688 -0.00826 -0.04930

D26 3.11287 -0.00023 -0.01947 0.00467 -0.01481 3.09806

D27 3.09241 -0.00021 -0.01041 0.00203 -0.00838 3.08403

D28 -0.03687 -0.00033 -0.01474 -0.00018 -0.01492 -0.05179

D29 -0.12386 0.00000 -0.02272 0.01380 -0.00894 -0.13280

D30 3.01191 0.00015 -0.01431 0.01586 0.00155 3.01346

D31 3.00542 0.00012 -0.01839 0.01600 -0.00240 3.00302

D32 -0.14199 0.00027 -0.00998 0.01806 0.00809 -0.13390

D33 -1.12686 0.00013 0.03273 -0.00967 0.02306 -1.10381

D34 2.01698 0.00010 0.03338 -0.01068 0.02269 2.03967

D35 2.02603 0.00001 0.02876 -0.01172 0.01704 2.04307

D36 -1.11332 -0.00003 0.02941 -0.01274 0.01668 -1.09664

D37 -3.12315 -0.00005 0.00987 -0.00879 0.00111 -3.12203

D38 0.02363 -0.00019 0.00241 -0.01063 -0.00822 0.01541

D39 3.13202 -0.00002 -0.00882 0.00445 -0.00439 3.12764

D40 -0.02646 0.00002 -0.00821 0.00525 -0.00297 -0.02943

D41 -0.01462 0.00011 -0.00152 0.00624 0.00471 -0.00991

D42 3.11009 0.00015 -0.00091 0.00703 0.00612 3.11621

D43 -0.02386 0.00020 -0.00240 0.01107 0.00867 -0.01519

D44 3.12372 0.00004 -0.01058 0.00887 -0.00175 3.12197

D45 0.01523 -0.00014 0.00149 -0.00742 -0.00591 0.00931

D46 -3.10952 -0.00016 0.00081 -0.00740 -0.00659 -3.11611

D47 -3.13219 0.00001 0.00950 -0.00528 0.00424 -3.12795

D48 0.02625 -0.00001 0.00882 -0.00526 0.00356 0.02981

D49 0.12098 0.00004 0.02470 -0.01328 0.01144 0.13242

D50 -3.01075 -0.00002 0.02195 -0.01399 0.00798 -3.00277

D51 -3.01389 -0.00013 0.01548 -0.01575 -0.00027 -3.01417

D52 0.13757 -0.00019 0.01273 -0.01646 -0.00373 0.13383

D53 -0.00036 0.00002 0.00001 0.00069 0.00070 0.00035

D54 -3.12484 -0.00001 -0.00060 -0.00011 -0.00071 -3.12556

D55 3.12417 0.00003 0.00070 0.00066 0.00137 3.12555

D56 -0.00031 -0.00000 0.00009 -0.00013 -0.00004 -0.00036

D57 -3.01191 -0.00015 0.01431 -0.01586 -0.00155 -3.01346

D58 0.12386 -0.00000 0.02272 -0.01380 0.00894 0.13280

D59 0.14199 -0.00027 0.00998 -0.01806 -0.00809 0.13390

D60 -3.00542 -0.00012 0.01839 -0.01600 0.00240 -3.00302

D61 1.12686 -0.00013 -0.03273 0.00967 -0.02306 1.10381

D62 -2.01698 -0.00010 -0.03338 0.01068 -0.02269 -2.03967

D63 -2.02603 -0.00001 -0.02876 0.01172 -0.01704 -2.04307

D64 1.11332 0.00003 -0.02941 0.01274 -0.01668 1.09664

D65 -3.13202 0.00002 0.00882 -0.00445 0.00439 -3.12764

D66 0.02646 -0.00002 0.00821 -0.00525 0.00297 0.02943

D67 0.01462 -0.00011 0.00152 -0.00624 -0.00471 0.00991

D68 -3.11009 -0.00015 0.00091 -0.00703 -0.00612 -3.11621

D69 3.12315 0.00005 -0.00987 0.00879 -0.00111 3.12203

D70 -0.02363 0.00019 -0.00241 0.01063 0.00822 -0.01541

D71 0.00036 -0.00002 -0.00001 -0.00069 -0.00070 -0.00035

D72 -3.12417 -0.00003 -0.00070 -0.00066 -0.00137 -3.12555

D73 3.12484 0.00001 0.00060 0.00011 0.00071 3.12556

D74 0.00031 0.00000 -0.00009 0.00013 0.00004 0.00036

D75 -0.01523 0.00014 -0.00149 0.00742 0.00591 -0.00931

D76 3.13219 -0.00001 -0.00950 0.00528 -0.00424 3.12795

D77 3.10952 0.00016 -0.00081 0.00740 0.00659 3.11611

D78 -0.02625 0.00001 -0.00882 0.00526 -0.00356 -0.02981

D79 0.02386 -0.00020 0.00240 -0.01107 -0.00867 0.01519

D80 -3.12372 -0.00004 0.01058 -0.00887 0.00175 -3.12197

D81 3.01389 0.00013 -0.01548 0.01575 0.00027 3.01417

D82 -0.13757 0.00019 -0.01273 0.01646 0.00373 -0.13383

D83 -0.12098 -0.00004 -0.02470 0.01328 -0.01144 -0.13242

D84 3.01075 0.00002 -0.02195 0.01399 -0.00798 3.00277

D85 3.09573 -0.00029 -0.01500 0.00182 -0.01318 3.08256

D86 -0.03869 -0.00018 -0.01709 0.00590 -0.01120 -0.04989

D87 -0.03599 -0.00035 -0.01775 0.00111 -0.01664 -0.05263

D88 3.11277 -0.00024 -0.01984 0.00519 -0.01467 3.09810

D89 -1.11085 -0.00007 0.03138 -0.01722 0.01416 -1.09669

D90 2.02804 -0.00003 0.03148 -0.01629 0.01519 2.04323

D91 2.02168 -0.00000 0.03390 -0.01655 0.01735 2.03904

D92 -1.12261 0.00004 0.03400 -0.01562 0.01838 -1.10423

D93 -3.13494 0.00002 -0.00818 0.00557 -0.00263 -3.13757

D94 -0.01064 0.00012 -0.00967 0.00922 -0.00047 -0.01111

D95 0.00071 -0.00007 -0.00645 0.00219 -0.00427 -0.00356

D96 3.12501 0.00003 -0.00794 0.00583 -0.00211 3.12290

D97 3.13447 0.00003 0.01254 -0.00704 0.00551 3.13999

D98 0.09042 -0.00020 -0.00225 -0.00455 -0.00679 0.08363

D99 -0.00119 0.00012 0.01081 -0.00366 0.00715 0.00596

D100 -3.04524 -0.00011 -0.00397 -0.00118 -0.00515 -3.05039

D101 -0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D102 3.12383 0.00010 -0.00154 0.00372 0.00220 3.12603

D103 -3.12383 -0.00010 0.00154 -0.00372 -0.00220 -3.12603

D104 0.00000 0.00000 -0.00000 0.00000 0.00000 0.00000

D105 -0.00071 0.00007 0.00645 -0.00219 0.00427 0.00356

D106 3.13494 -0.00002 0.00818 -0.00557 0.00263 3.13757

D107 -3.12501 -0.00003 0.00794 -0.00583 0.00211 -3.12290

D108 0.01064 -0.00012 0.00967 -0.00922 0.00047 0.01111

D109 0.00119 -0.00012 -0.01081 0.00366 -0.00715 -0.00596

D110 3.04524 0.00011 0.00397 0.00118 0.00515 3.05039

D111 -3.13447 -0.00003 -0.01254 0.00704 -0.00551 -3.13999

D112 -0.09042 0.00020 0.00225 0.00455 0.00679 -0.08363

D113 -3.09573 0.00029 0.01500 -0.00182 0.01318 -3.08256

D114 0.03599 0.00035 0.01775 -0.00111 0.01664 0.05263

D115 0.03869 0.00018 0.01709 -0.00590 0.01120 0.04989

D116 -3.11277 0.00024 0.01984 -0.00519 0.01467 -3.09810

D117 1.11085 0.00007 -0.03138 0.01722 -0.01416 1.09669

D118 -2.02804 0.00003 -0.03148 0.01629 -0.01519 -2.04323

D119 -2.02168 0.00000 -0.03390 0.01655 -0.01735 -2.03904

D120 1.12261 -0.00004 -0.03400 0.01562 -0.01838 1.10423

D121 3.13636 -0.00000 0.00034 -0.00042 -0.00008 3.13628

D122 -0.01556 0.00007 -0.00015 0.00244 0.00229 -0.01326

D123 -0.00743 0.00003 -0.00029 0.00057 0.00028 -0.00715

D124 3.12384 0.00010 -0.00078 0.00343 0.00265 3.12649

D125 -3.13788 0.00006 0.00029 0.00107 0.00136 -3.13652

D126 -0.00576 0.00007 -0.00088 0.00261 0.00172 -0.00403

D127 0.00589 0.00003 0.00092 0.00009 0.00101 0.00689

D128 3.13801 0.00004 -0.00025 0.00163 0.00137 3.13938

D129 0.00477 -0.00006 -0.00035 -0.00088 -0.00123 0.00354

D130 3.14042 -0.00002 -0.00119 0.00046 -0.00073 3.13969

D131 -3.12646 -0.00013 0.00015 -0.00375 -0.00360 -3.13006

D132 0.00919 -0.00009 -0.00069 -0.00241 -0.00310 0.00609

D133 -0.00035 0.00003 0.00037 0.00050 0.00087 0.00051

D134 3.14011 0.00004 0.00014 0.00067 0.00081 3.14092

D135 -3.13597 -0.00001 0.00121 -0.00084 0.00036 -3.13561

D136 0.00449 -0.00000 0.00098 -0.00067 0.00031 0.00480

D137 -0.00118 0.00002 0.00026 0.00015 0.00041 -0.00077

D138 -3.13879 0.00001 0.00095 -0.00033 0.00062 -3.13817

D139 3.14155 0.00002 0.00048 -0.00002 0.00046 -3.14118

D140 0.00393 0.00001 0.00118 -0.00050 0.00068 0.00461

D141 -0.00166 -0.00005 -0.00091 -0.00044 -0.00136 -0.00302

D142 -3.13374 -0.00006 0.00027 -0.00199 -0.00172 -3.13546

D143 3.13597 -0.00004 -0.00161 0.00004 -0.00157 3.13440

D144 0.00389 -0.00006 -0.00042 -0.00151 -0.00193 0.00196

D145 0.00035 -0.00003 -0.00037 -0.00050 -0.00087 -0.00051

D146 3.13597 0.00001 -0.00121 0.00084 -0.00036 3.13561

D147 -3.14011 -0.00004 -0.00014 -0.00067 -0.00081 -3.14092

D148 -0.00449 0.00000 -0.00098 0.00067 -0.00031 -0.00480

D149 0.00118 -0.00002 -0.00026 -0.00015 -0.00041 0.00077

D150 3.13879 -0.00001 -0.00095 0.00033 -0.00062 3.13817

D151 -3.14155 -0.00002 -0.00048 0.00002 -0.00046 3.14118

D152 -0.00393 -0.00001 -0.00118 0.00050 -0.00068 -0.00461

D153 -0.00477 0.00006 0.00035 0.00088 0.00123 -0.00354

D154 3.12646 0.00013 -0.00015 0.00375 0.00360 3.13006

D155 -3.14042 0.00002 0.00119 -0.00046 0.00073 -3.13969

D156 -0.00919 0.00009 0.00069 0.00241 0.00310 -0.00609

D157 -3.13636 0.00000 -0.00034 0.00042 0.00008 -3.13628

D158 0.00743 -0.00003 0.00029 -0.00057 -0.00028 0.00715

D159 0.01556 -0.00007 0.00015 -0.00244 -0.00229 0.01326

D160 -3.12384 -0.00010 0.00078 -0.00343 -0.00265 -3.12649

D161 3.13788 -0.00006 -0.00029 -0.00107 -0.00136 3.13652

D162 0.00576 -0.00007 0.00088 -0.00261 -0.00172 0.00403

D163 -0.00589 -0.00003 -0.00092 -0.00009 -0.00101 -0.00689

D164 -3.13801 -0.00004 0.00025 -0.00163 -0.00137 -3.13938

D165 0.00166 0.00005 0.00091 0.00044 0.00136 0.00302

D166 -3.13597 0.00004 0.00161 -0.00004 0.00157 -3.13440

D167 3.13374 0.00006 -0.00027 0.00199 0.00172 3.13546

D168 -0.00389 0.00006 0.00042 0.00151 0.00193 -0.00196

D169 3.13824 -0.00007 -0.00109 -0.00094 -0.00203 3.13621

D170 0.00585 -0.00006 0.00045 -0.00225 -0.00181 0.00404

D171 -0.00597 -0.00003 -0.00099 -0.00005 -0.00104 -0.00701

D172 -3.13836 -0.00003 0.00054 -0.00136 -0.00081 -3.13917

D173 -3.13633 -0.00000 0.00034 -0.00005 0.00029 -3.13604

D174 0.01585 -0.00007 0.00070 -0.00267 -0.00197 0.01388

D175 0.00790 -0.00004 0.00024 -0.00095 -0.00071 0.00719

D176 -3.12311 -0.00011 0.00060 -0.00357 -0.00297 -3.12608

D177 0.00136 0.00006 0.00106 0.00071 0.00177 0.00312

D178 -3.13618 0.00005 0.00179 0.00011 0.00190 -3.13428

D179 3.13370 0.00006 -0.00049 0.00202 0.00154 3.13524

D180 -0.00384 0.00005 0.00024 0.00142 0.00167 -0.00217

D181 0.00151 -0.00003 -0.00035 -0.00039 -0.00074 0.00076

D182 -3.14135 -0.00002 -0.00052 -0.00013 -0.00065 3.14119

D183 3.13902 -0.00002 -0.00108 0.00021 -0.00087 3.13815

D184 -0.00383 -0.00001 -0.00125 0.00047 -0.00078 -0.00461

D185 0.00040 -0.00004 -0.00039 -0.00059 -0.00098 -0.00058

D186 3.13578 0.00001 -0.00117 0.00095 -0.00023 3.13555

D187 -3.13993 -0.00005 -0.00023 -0.00085 -0.00108 -3.14101

D188 -0.00455 0.00000 -0.00101 0.00069 -0.00032 -0.00488

D189 -0.00522 0.00008 0.00044 0.00129 0.00174 -0.00348

D190 3.12574 0.00014 0.00008 0.00392 0.00400 3.12974

D191 -3.14063 0.00003 0.00123 -0.00024 0.00099 -3.13964

D192 -0.00968 0.00010 0.00087 0.00239 0.00326 -0.00642

D193 -3.13824 0.00007 0.00109 0.00094 0.00203 -3.13621

D194 -0.00585 0.00006 -0.00045 0.00225 0.00181 -0.00404

D195 0.00597 0.00003 0.00099 0.00005 0.00104 0.00701

D196 3.13836 0.00003 -0.00054 0.00136 0.00081 3.13917

D197 3.13633 0.00000 -0.00034 0.00005 -0.00029 3.13604

D198 -0.01585 0.00007 -0.00070 0.00267 0.00197 -0.01388

D199 -0.00790 0.00004 -0.00024 0.00095 0.00071 -0.00719

D200 3.12311 0.00011 -0.00060 0.00357 0.00297 3.12608

D201 -0.00136 -0.00006 -0.00106 -0.00071 -0.00177 -0.00312

D202 3.13618 -0.00005 -0.00179 -0.00011 -0.00190 3.13428

D203 -3.13370 -0.00006 0.00049 -0.00202 -0.00154 -3.13524

D204 0.00384 -0.00005 -0.00024 -0.00142 -0.00167 0.00217

D205 -0.00151 0.00003 0.00035 0.00039 0.00074 -0.00076

D206 3.14135 0.00002 0.00052 0.00013 0.00065 -3.14119

D207 -3.13902 0.00002 0.00108 -0.00021 0.00087 -3.13815

D208 0.00383 0.00001 0.00125 -0.00047 0.00078 0.00461

D209 -0.00040 0.00004 0.00039 0.00059 0.00098 0.00058

D210 -3.13578 -0.00001 0.00117 -0.00095 0.00023 -3.13555

D211 3.13993 0.00005 0.00023 0.00085 0.00108 3.14101

D212 0.00455 -0.00000 0.00101 -0.00069 0.00032 0.00488

D213 0.00522 -0.00008 -0.00044 -0.00129 -0.00174 0.00348

D214 -3.12574 -0.00014 -0.00008 -0.00392 -0.00400 -3.12974

D215 3.14063 -0.00003 -0.00123 0.00024 -0.00099 3.13964

D216 0.00968 -0.00010 -0.00087 -0.00239 -0.00326 0.00642

Item Value Threshold Converged?

Maximum Force 0.003719 0.000450 NO

RMS Force 0.000583 0.000300 NO

Maximum Displacement 0.108389 0.001800 NO

RMS Displacement 0.029825 0.001200 NO

Predicted change in Energy=-1.777867D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Aug 18 14:21:13 2019, MaxMem= 2013265920 cpu: 1.4

(Enter /home/kira/g09/l202.exe)

Stoichiometry C44H30N4(1-,2)

Framework group CS[SG(H2N2),X(C44H28N2)]

Deg. of freedom 116

Full point group CS NOp 2

RotChk: IX=3 Diff= 5.04D-06

Largest Abelian subgroup CS NOp 2

Largest concise Abelian subgroup CS NOp 2

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 4.260423 -0.144497 0.680272

2 6 0 2.899556 -0.001837 1.143492

3 7 0 2.118708 0.076147 -0.000000

4 6 0 2.899556 -0.001837 -1.143492

5 6 0 4.260423 -0.144497 -0.680272

6 6 0 2.461926 0.039643 -2.455980

7 6 0 1.095443 0.115662 -2.874389

8 7 0 0.000088 0.012061 -2.054585

9 6 0 -1.095171 0.115945 -2.874542

10 6 0 -0.687390 0.309245 -4.239697

11 6 0 0.688040 0.309362 -4.239535

12 6 0 2.461926 0.039643 2.455980

13 6 0 1.095443 0.115662 2.874389

14 6 0 0.688040 0.309362 4.239535

15 6 0 -0.687390 0.309245 4.239697

16 6 0 -1.095171 0.115945 2.874542

17 7 0 0.000088 0.012061 2.054585

18 6 0 -2.461720 0.040189 2.456212

19 6 0 -2.899323 -0.001692 1.143532

20 6 0 -4.260033 -0.145793 0.680263

21 6 0 -4.260033 -0.145793 -0.680263

22 6 0 -2.899323 -0.001692 -1.143532

23 7 0 -2.118639 0.076206 0.000000

24 6 0 -2.461720 0.040189 -2.456212

25 6 0 3.502524 -0.005750 -3.524141

26 6 0 4.454856 1.013441 -3.654058

27 6 0 5.428158 0.961631 -4.650332

28 6 0 5.464412 -0.110904 -5.539763

29 6 0 4.518984 -1.130520 -5.424821

30 6 0 3.548244 -1.076090 -4.428476

31 6 0 5.464412 -0.110904 5.539763

32 6 0 5.428158 0.961631 4.650332

33 6 0 4.454856 1.013441 3.654058

34 6 0 3.502524 -0.005750 3.524141

35 6 0 3.548244 -1.076090 4.428476

36 6 0 4.518984 -1.130520 5.424821

37 6 0 -3.502402 -0.005280 -3.524185

38 6 0 -3.548556 -1.075804 -4.428385

39 6 0 -4.519650 -1.130468 -5.424337

40 6 0 -5.465095 -0.110866 -5.539271

41 6 0 -5.428421 0.961893 -4.650130

42 6 0 -4.454825 1.013900 -3.654181

43 6 0 -3.502402 -0.005280 3.524185

44 6 0 -3.548556 -1.075804 4.428385

45 6 0 -4.519650 -1.130468 5.424337

46 6 0 -5.465095 -0.110866 5.539271

47 6 0 -5.428421 0.961893 4.650130

48 6 0 -4.454825 1.013900 3.654181

49 1 0 5.118443 -0.246803 1.326075

50 1 0 5.118443 -0.246803 -1.326075

51 1 0 -1.341594 0.443582 -5.088601

52 1 0 1.342531 0.443498 -5.088270

53 1 0 1.342531 0.443498 5.088270

54 1 0 -1.341594 0.443582 5.088601

55 1 0 -5.117873 -0.250164 1.325941

56 1 0 -5.117873 -0.250164 -1.325941

57 1 0 4.425881 1.856540 -2.971922

58 1 0 6.154906 1.763406 -4.733409

59 1 0 6.221211 -0.152157 -6.316211

60 1 0 4.539580 -1.972089 -6.109842

61 1 0 2.819803 -1.875102 -4.341302

62 1 0 6.221211 -0.152157 6.316211

63 1 0 6.154906 1.763406 4.733409

64 1 0 4.425881 1.856540 2.971922

65 1 0 2.819803 -1.875102 4.341302

66 1 0 4.539580 -1.972089 6.109842

67 1 0 -2.820306 -1.874969 -4.341205

68 1 0 -4.540500 -1.972259 -6.109079

69 1 0 -6.222183 -0.152316 -6.315423

70 1 0 -6.155104 1.763734 -4.733157

71 1 0 -4.425467 1.857369 -2.972544

72 1 0 -2.820306 -1.874969 4.341205

73 1 0 -4.540500 -1.972259 6.109079

74 1 0 -6.222183 -0.152316 6.315423

75 1 0 -6.155104 1.763734 4.733157

76 1 0 -4.425467 1.857369 2.972544

77 1 0 1.108228 0.097610 -0.000000

78 1 0 -1.108371 0.105623 0.000000

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

Rotational constants (GHZ): 0.0584998 0.0577331 0.0300064

Leave Link 202 at Sun Aug 18 14:21:13 2019, MaxMem= 2013265920 cpu: 0.1

(Enter /home/kira/g09/l301.exe)

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

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

There are 513 symmetry adapted cartesian basis functions of A' symmetry.

There are 489 symmetry adapted cartesian basis functions of A" symmetry.

There are 488 symmetry adapted basis functions of A' symmetry.

There are 466 symmetry adapted basis functions of A" symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 161 beta electrons

nuclear repulsion energy 5346.4586456916 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= 78 NActive= 78 NUniq= 41 SFac= 3.62D+00 NAtFMM= 60 NAOKFM=T 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= -0.2117882292 Hartrees.

Nuclear repulsion after empirical dispersion term = 5346.2468574624 Hartrees.

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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= 78.

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

Smoothing algorithm: York/Karplus (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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5726

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.32D-09

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 300

GePol: Fraction of low-weight points (<1% of avg) = 5.24%

GePol: Cavity surface area = 616.979 Ang\*\*2

GePol: Cavity volume = 628.765 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0020092138 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5346.2448482486 Hartrees.

Leave Link 301 at Sun Aug 18 14:21:13 2019, MaxMem= 2013265920 cpu: 1.2

(Enter /home/kira/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.

One-electron integral symmetry used in STVInt

NBasis= 954 RedAO= T EigKep= 9.03D-05 NBF= 488 466

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 488 466

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= 938 938 939 939 940 MxSgAt= 78 MxSgA2= 78.

Leave Link 302 at Sun Aug 18 14:21:15 2019, MaxMem= 2013265920 cpu: 10.3

(Enter /home/kira/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sun Aug 18 14:21:15 2019, MaxMem= 2013265920 cpu: 1.2

(Enter /home/kira/g09/l401.exe)

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

B after Tr= 0.000000 -0.000000 0.000000

Rot= 1.000000 0.000000 -0.000000 0.000040 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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The electronic state of the initial guess is 2-A'.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7585 S= 0.5043

Generating alternative initial guess.

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2000

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= -1914.57967940382

Leave Link 401 at Sun Aug 18 14:21:21 2019, MaxMem= 2013265920 cpu: 48.3

(Enter /home/kira/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3047318 IEndB= 3047318 NGot= 2013265920 MDV= 2011240249

LenX= 2011240249 LenY= 2010235243

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= 480000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 98361228.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.11D-15 for 5716.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.00D-15 for 5723 159.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.33D-15 for 5716.

Iteration 1 A^-1\*A deviation from orthogonality is 1.31D-12 for 3430 3424.

E= -1914.48728899117

DIIS: error= 2.64D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.48728899117 IErMin= 1 ErrMin= 2.64D-03

ErrMax= 2.64D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.20D-02 BMatP= 1.20D-02

IDIUse=3 WtCom= 9.74D-01 WtEn= 2.64D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.446 Goal= None Shift= 0.000

Gap= 0.504 Goal= None Shift= 0.000

GapD= 0.446 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=8.06D-05 MaxDP=2.50D-03 OVMax= 1.32D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 8.06D-05 CP: 1.00D+00

E= -1914.49341141142 Delta-E= -0.006122420250 Rises=F Damp=F

DIIS: error= 3.61D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.49341141142 IErMin= 2 ErrMin= 3.61D-04

ErrMax= 3.61D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.98D-04 BMatP= 1.20D-02

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.61D-03

Coeff-Com: -0.616D-01 0.106D+01

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

Coeff: -0.614D-01 0.106D+01

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=1.56D-05 MaxDP=6.01D-04 DE=-6.12D-03 OVMax= 2.38D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.47D-05 CP: 1.00D+00 1.06D+00

E= -1914.49348963946 Delta-E= -0.000078228039 Rises=F Damp=F

DIIS: error= 2.16D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.49348963946 IErMin= 3 ErrMin= 2.16D-04

ErrMax= 2.16D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.43D-04 BMatP= 1.98D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.16D-03

Coeff-Com: -0.392D-01 0.520D+00 0.519D+00

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

Coeff: -0.391D-01 0.519D+00 0.520D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=7.52D-06 MaxDP=5.25D-04 DE=-7.82D-05 OVMax= 1.59D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 5.92D-06 CP: 1.00D+00 1.08D+00 7.00D-01

E= -1914.49351691448 Delta-E= -0.000027275018 Rises=F Damp=F

DIIS: error= 9.77D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.49351691448 IErMin= 4 ErrMin= 9.77D-05

ErrMax= 9.77D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.39D-05 BMatP= 1.43D-04

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

Coeff-Com: -0.110D-01 0.114D+00 0.299D+00 0.598D+00

Coeff: -0.110D-01 0.114D+00 0.299D+00 0.598D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=3.06D-06 MaxDP=1.88D-04 DE=-2.73D-05 OVMax= 7.05D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.87D-06 CP: 1.00D+00 1.08D+00 7.79D-01 6.50D-01

E= -1914.49352208960 Delta-E= -0.000005175119 Rises=F Damp=F

DIIS: error= 2.55D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.49352208960 IErMin= 5 ErrMin= 2.55D-05

ErrMax= 2.55D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.80D-06 BMatP= 2.39D-05

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

Coeff-Com: -0.212D-02 0.102D-01 0.101D+00 0.294D+00 0.597D+00

Coeff: -0.212D-02 0.102D-01 0.101D+00 0.294D+00 0.597D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=1.07D-06 MaxDP=6.70D-05 DE=-5.18D-06 OVMax= 2.45D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 6.86D-07 CP: 1.00D+00 1.08D+00 7.75D-01 7.51D-01 7.12D-01

E= -1914.49352246076 Delta-E= -0.000000371166 Rises=F Damp=F

DIIS: error= 1.21D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.49352246076 IErMin= 6 ErrMin= 1.21D-05

ErrMax= 1.21D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.71D-07 BMatP= 1.80D-06

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

Coeff-Com: 0.763D-03-0.157D-01 0.289D-02 0.595D-01 0.349D+00 0.603D+00

Coeff: 0.763D-03-0.157D-01 0.289D-02 0.595D-01 0.349D+00 0.603D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=4.28D-07 MaxDP=2.50D-05 DE=-3.71D-07 OVMax= 9.02D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.53D-07 CP: 1.00D+00 1.08D+00 7.90D-01 7.38D-01 7.91D-01

CP: 5.78D-01

E= -1914.49352255263 Delta-E= -0.000000091873 Rises=F Damp=F

DIIS: error= 2.70D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.49352255263 IErMin= 7 ErrMin= 2.70D-06

ErrMax= 2.70D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.61D-08 BMatP= 3.71D-07

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

Coeff-Com: 0.459D-03-0.853D-02-0.137D-02 0.233D-01 0.168D+00 0.323D+00

Coeff-Com: 0.495D+00

Coeff: 0.459D-03-0.853D-02-0.137D-02 0.233D-01 0.168D+00 0.323D+00

Coeff: 0.495D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=9.01D-08 MaxDP=5.83D-06 DE=-9.19D-08 OVMax= 1.98D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 6.93D-08 CP: 1.00D+00 1.08D+00 7.89D-01 7.43D-01 7.85D-01

CP: 6.34D-01 8.41D-01

E= -1914.49352255653 Delta-E= -0.000000003897 Rises=F Damp=F

DIIS: error= 9.64D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.49352255653 IErMin= 8 ErrMin= 9.64D-07

ErrMax= 9.64D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.13D-09 BMatP= 1.61D-08

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

Coeff-Com: 0.120D-05 0.411D-03-0.152D-02-0.559D-02-0.184D-01-0.129D-01

Coeff-Com: 0.225D+00 0.813D+00

Coeff: 0.120D-05 0.411D-03-0.152D-02-0.559D-02-0.184D-01-0.129D-01

Coeff: 0.225D+00 0.813D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=4.39D-08 MaxDP=2.65D-06 DE=-3.90D-09 OVMax= 1.35D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 3.00D-08 CP: 1.00D+00 1.08D+00 7.89D-01 7.43D-01 7.88D-01

CP: 6.40D-01 1.04D+00 1.02D+00

E= -1914.49352255774 Delta-E= -0.000000001211 Rises=F Damp=F

DIIS: error= 8.00D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.49352255774 IErMin= 9 ErrMin= 8.00D-07

ErrMax= 8.00D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.78D-10 BMatP= 2.13D-09

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

Coeff-Com: -0.845D-04 0.180D-02-0.452D-03-0.702D-02-0.408D-01-0.667D-01

Coeff-Com: 0.177D-01 0.396D+00 0.700D+00

Coeff: -0.845D-04 0.180D-02-0.452D-03-0.702D-02-0.408D-01-0.667D-01

Coeff: 0.177D-01 0.396D+00 0.700D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=2.55D-08 MaxDP=1.68D-06 DE=-1.21D-09 OVMax= 9.36D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.73D-08 CP: 1.00D+00 1.08D+00 7.89D-01 7.43D-01 7.90D-01

CP: 6.47D-01 1.10D+00 1.24D+00 1.03D+00

E= -1914.49352255808 Delta-E= -0.000000000339 Rises=F Damp=F

DIIS: error= 5.54D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.49352255808 IErMin=10 ErrMin= 5.54D-07

ErrMax= 5.54D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.05D-10 BMatP= 5.78D-10

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

Coeff-Com: -0.445D-04 0.768D-03 0.414D-03-0.132D-02-0.142D-01-0.298D-01

Coeff-Com: -0.815D-01-0.133D+00 0.386D+00 0.873D+00

Coeff: -0.445D-04 0.768D-03 0.414D-03-0.132D-02-0.142D-01-0.298D-01

Coeff: -0.815D-01-0.133D+00 0.386D+00 0.873D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=1.95D-08 MaxDP=1.14D-06 DE=-3.39D-10 OVMax= 6.25D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 9.55D-09 CP: 1.00D+00 1.08D+00 7.89D-01 7.43D-01 7.90D-01

CP: 6.50D-01 1.16D+00 1.31D+00 1.43D+00 1.21D+00

E= -1914.49352255827 Delta-E= -0.000000000188 Rises=F Damp=F

DIIS: error= 2.45D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.49352255827 IErMin=11 ErrMin= 2.45D-07

ErrMax= 2.45D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.09D-11 BMatP= 2.05D-10

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

Coeff-Com: 0.394D-05-0.177D-03 0.348D-03 0.148D-02 0.525D-02 0.588D-02

Coeff-Com: -0.422D-01-0.172D+00-0.178D-01 0.407D+00 0.812D+00

Coeff: 0.394D-05-0.177D-03 0.348D-03 0.148D-02 0.525D-02 0.588D-02

Coeff: -0.422D-01-0.172D+00-0.178D-01 0.407D+00 0.812D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=8.93D-09 MaxDP=4.33D-07 DE=-1.88D-10 OVMax= 2.81D-06

Error on total polarization charges = 0.08609

SCF Done: E(UB3LYP) = -1914.49352256 A.U. after 11 cycles

NFock= 11 Conv=0.89D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7585 S= 0.5043

<L.S>= 0.000000000000E+00

KE= 1.906557357164D+03 PE=-1.517740353414D+04 EE= 6.010107806172D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.26

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7585, after 0.7500

Leave Link 502 at Sun Aug 18 14:27:59 2019, MaxMem= 2013265920 cpu: 3164.9

(Enter /home/kira/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 = 186

Leave Link 701 at Sun Aug 18 14:28:16 2019, MaxMem= 2013265920 cpu: 138.4

(Enter /home/kira/g09/l702.exe)

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

Leave Link 702 at Sun Aug 18 14:28:16 2019, MaxMem= 2013265920 cpu: 0.2

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 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= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

Petite list used in FoFCou.

Leave Link 703 at Sun Aug 18 14:29:30 2019, MaxMem= 2013265920 cpu: 591.0

(Enter /home/kira/g09/l716.exe)

Dipole =-2.52942098D-04-1.50511377D-01-5.79980508D-13

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000604308 -0.000091781 0.001341908

2 6 0.000865272 0.000206877 -0.002335727

3 7 0.000660775 -0.000556208 0.000000000

4 6 0.000865272 0.000206877 0.002335727

5 6 -0.000604308 -0.000091781 -0.001341908

6 6 -0.000728912 -0.000123640 -0.000812594

7 6 -0.000022189 -0.000543450 -0.000847101

8 7 -0.000008035 0.000908416 0.000374430

9 6 0.000023916 -0.000578442 -0.000874147

10 6 -0.000450770 0.000185496 0.000362689

11 6 0.000416940 0.000111213 0.000336081

12 6 -0.000728912 -0.000123640 0.000812594

13 6 -0.000022189 -0.000543450 0.000847101

14 6 0.000416940 0.000111213 -0.000336081

15 6 -0.000450770 0.000185496 -0.000362689

16 6 0.000023916 -0.000578442 0.000874147

17 7 -0.000008035 0.000908416 -0.000374430

18 6 0.000758524 -0.000141758 0.000681379

19 6 -0.000862619 0.000208637 -0.002251474

20 6 0.000616993 -0.000126629 0.001374566

21 6 0.000616993 -0.000126629 -0.001374566

22 6 -0.000862619 0.000208637 0.002251474

23 7 -0.000602089 -0.000431142 -0.000000000

24 6 0.000758524 -0.000141758 -0.000681379

25 6 0.000527560 0.000123578 -0.000401824

26 6 -0.000240387 0.000243162 0.000352212

27 6 0.000055368 -0.000053987 -0.000170877

28 6 -0.000121229 0.000024361 0.000126893

29 6 0.000175712 0.000032440 -0.000073462

30 6 -0.000302012 -0.000291385 0.000230555

31 6 -0.000121229 0.000024361 -0.000126893

32 6 0.000055368 -0.000053987 0.000170877

33 6 -0.000240387 0.000243162 -0.000352212

34 6 0.000527560 0.000123578 0.000401824

35 6 -0.000302012 -0.000291385 -0.000230555

36 6 0.000175712 0.000032440 0.000073462

37 6 -0.000608781 0.000123275 -0.000488876

38 6 0.000326781 -0.000275144 0.000291492

39 6 -0.000186494 0.000032914 -0.000091325

40 6 0.000131760 0.000024584 0.000140666

41 6 -0.000070562 -0.000054958 -0.000182016

42 6 0.000300679 0.000235143 0.000371001

43 6 -0.000608781 0.000123275 0.000488876

44 6 0.000326781 -0.000275144 -0.000291492

45 6 -0.000186494 0.000032914 0.000091325

46 6 0.000131760 0.000024584 -0.000140666

47 6 -0.000070562 -0.000054958 0.000182016

48 6 0.000300679 0.000235143 -0.000371001

49 1 -0.000075258 0.000033007 -0.000035697

50 1 -0.000075258 0.000033007 0.000035697

51 1 0.000079687 -0.000008723 0.000072655

52 1 -0.000102819 -0.000008316 0.000079106

53 1 -0.000102819 -0.000008316 -0.000079106

54 1 0.000079687 -0.000008723 -0.000072655

55 1 0.000067286 0.000056890 -0.000010019

56 1 0.000067286 0.000056890 0.000010019

57 1 -0.000006536 -0.000093049 -0.000020767

58 1 -0.000028098 -0.000012540 -0.000059140

59 1 0.000004891 -0.000002429 -0.000004156

60 1 0.000060773 0.000011407 0.000027628

61 1 0.000054490 0.000093304 0.000007006

62 1 0.000004891 -0.000002429 0.000004156

63 1 -0.000028098 -0.000012540 0.000059140

64 1 -0.000006536 -0.000093049 0.000020767

65 1 0.000054490 0.000093304 -0.000007006

66 1 0.000060773 0.000011407 -0.000027628

67 1 -0.000037352 0.000090821 0.000006892

68 1 -0.000061520 0.000012964 0.000027027

69 1 -0.000004604 -0.000001463 -0.000004669

70 1 0.000027486 -0.000013548 -0.000060829

71 1 -0.000000658 -0.000095762 0.000004976

72 1 -0.000037352 0.000090821 -0.000006892

73 1 -0.000061520 0.000012964 -0.000027027

74 1 -0.000004604 -0.000001463 0.000004669

75 1 0.000027486 -0.000013548 0.000060829

76 1 -0.000000658 -0.000095762 -0.000004976

77 1 0.000003391 0.000305848 0.000000000

78 1 -0.000004026 0.000198528 -0.000000000

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

Cartesian Forces: Max 0.002335727 RMS 0.000468875

Leave Link 716 at Sun Aug 18 14:29:30 2019, MaxMem= 2013265920 cpu: 0.2

(Enter /home/kira/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 0.001168628 RMS 0.000201412

Search for a local minimum.

Step number 5 out of a maximum of 452

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

RMS Force = .20141D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 2 3 4 5

DE= -2.14D-04 DEPred=-1.78D-04 R= 1.20D+00

TightC=F SS= 1.41D+00 RLast= 1.07D-01 DXNew= 1.6128D+00 3.2225D-01

Trust test= 1.20D+00 RLast= 1.07D-01 DXMaxT set to 9.59D-01

ITU= 1 1 1 1 0

Eigenvalues --- 0.00441 0.00983 0.00988 0.00991 0.01405

Eigenvalues --- 0.01615 0.01616 0.01621 0.01639 0.01659

Eigenvalues --- 0.01722 0.01722 0.01722 0.01727 0.01737

Eigenvalues --- 0.01752 0.01757 0.01775 0.01788 0.01793

Eigenvalues --- 0.01837 0.01849 0.01855 0.01891 0.01901

Eigenvalues --- 0.01926 0.01929 0.01943 0.01965 0.01988

Eigenvalues --- 0.02003 0.02013 0.02020 0.02027 0.02068

Eigenvalues --- 0.02068 0.02070 0.02070 0.02077 0.02083

Eigenvalues --- 0.02104 0.02111 0.02118 0.02118 0.02119

Eigenvalues --- 0.02129 0.02130 0.02131 0.02132 0.02132

Eigenvalues --- 0.02132 0.02145 0.02160 0.02160 0.02160

Eigenvalues --- 0.02160 0.02162 0.02162 0.02162 0.02173

Eigenvalues --- 0.02173 0.02173 0.02175 0.02176 0.02181

Eigenvalues --- 0.02181 0.02181 0.02185 0.02186 0.02187

Eigenvalues --- 0.02187 0.02199 0.02216 0.02217 0.03463

Eigenvalues --- 0.15896 0.15916 0.15948 0.15996 0.15996

Eigenvalues --- 0.15996 0.15997 0.15998 0.15998 0.15999

Eigenvalues --- 0.15999 0.15999 0.15999 0.15999 0.15999

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16001 0.16007 0.16079

Eigenvalues --- 0.21991 0.22000 0.22000 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22000 0.22418 0.22756

Eigenvalues --- 0.22771 0.22814 0.22835 0.23471 0.23471

Eigenvalues --- 0.23476 0.23542 0.23749 0.24503 0.24727

Eigenvalues --- 0.24808 0.24815 0.24974 0.24989 0.24999

Eigenvalues --- 0.24999 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25068

Eigenvalues --- 0.25693 0.27267 0.34159 0.34182 0.34206

Eigenvalues --- 0.34529 0.35412 0.35413 0.35413 0.35413

Eigenvalues --- 0.35415 0.35415 0.35416 0.35416 0.35416

Eigenvalues --- 0.35416 0.35416 0.35422 0.35506 0.35507

Eigenvalues --- 0.35508 0.35523 0.35542 0.35545 0.35547

Eigenvalues --- 0.35688 0.36056 0.36057 0.36058 0.36105

Eigenvalues --- 0.36250 0.36250 0.36251 0.36282 0.37124

Eigenvalues --- 0.37164 0.37259 0.37293 0.38176 0.39128

Eigenvalues --- 0.39744 0.39871 0.40257 0.40414 0.40462

Eigenvalues --- 0.40629 0.41772 0.41789 0.41804 0.41878

Eigenvalues --- 0.42084 0.42085 0.42088 0.42095 0.42939

Eigenvalues --- 0.43279 0.44660 0.45420 0.45569 0.45570

Eigenvalues --- 0.45586 0.45586 0.45702 0.45770 0.45837

Eigenvalues --- 0.45845 0.45930 0.45939 0.45942 0.45947

Eigenvalues --- 0.45969 0.46660 0.46661 0.46661 0.46668

Eigenvalues --- 0.47073 0.47079 0.47086 0.47306 0.47578

Eigenvalues --- 0.48192 0.48280 0.49336 0.49432 0.49974

Eigenvalues --- 0.50771 0.50809 0.54861

En-DIIS/RFO-DIIS IScMMF= 0 using points: 5 4 3 2

RFO step: Lambda=-4.76509964D-05.

NNeg= 0 NP= 4 Switch= 2.50D-03 Rises=F DC= 4.14D-04 SmlDif= 1.00D-05

RMS Error= 0.7803412875D-03 NUsed= 4 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.87034 -0.25128 -0.81232 0.19327

Iteration 1 RMS(Cart)= 0.06342745 RMS(Int)= 0.00102843

Iteration 2 RMS(Cart)= 0.00187885 RMS(Int)= 0.00007463

Iteration 3 RMS(Cart)= 0.00000181 RMS(Int)= 0.00007463

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00007463

ITry= 1 IFail=0 DXMaxC= 2.33D-01 DCOld= 1.00D+10 DXMaxT= 9.59D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 2.28D-08 for atom 62.

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

(Linear) (Quad) (Total)

R1 2.72991 -0.00082 -0.00075 -0.00215 -0.00287 2.72704

R2 2.57106 0.00071 0.00024 0.00235 0.00268 2.57374

R3 2.03856 -0.00008 -0.00004 -0.00003 -0.00007 2.03849

R4 2.62078 -0.00076 -0.00113 -0.00157 -0.00278 2.61801

R5 2.61566 0.00117 0.00188 0.00100 0.00288 2.61854

R6 2.62078 -0.00076 -0.00113 -0.00157 -0.00278 2.61801

R7 1.90996 0.00000 0.00001 0.00008 0.00009 1.91006

R8 2.72991 -0.00082 -0.00075 -0.00215 -0.00287 2.72704

R9 2.61566 0.00117 0.00188 0.00100 0.00288 2.61854

R10 2.03856 -0.00008 -0.00004 -0.00003 -0.00007 2.03849

R11 2.70444 0.00005 0.00075 -0.00221 -0.00146 2.70298

R12 2.81935 0.00011 0.00068 0.00111 0.00179 2.82114

R13 2.59286 0.00005 -0.00037 0.00009 -0.00037 2.59249

R14 2.71695 -0.00037 -0.00056 -0.00067 -0.00120 2.71575

R15 2.59293 0.00005 -0.00036 0.00008 -0.00035 2.59258

R16 2.71707 -0.00043 -0.00052 -0.00098 -0.00147 2.71560

R17 2.70448 -0.00002 0.00070 -0.00253 -0.00183 2.70266

R18 2.59919 0.00029 0.00073 0.00036 0.00120 2.60038

R19 2.04114 -0.00011 -0.00040 0.00019 -0.00021 2.04093

R20 2.04117 -0.00013 -0.00039 0.00008 -0.00031 2.04086

R21 2.70444 0.00005 0.00075 -0.00221 -0.00146 2.70298

R22 2.81935 0.00011 0.00068 0.00111 0.00179 2.82114

R23 2.71695 -0.00037 -0.00056 -0.00067 -0.00120 2.71575

R24 2.59286 0.00005 -0.00037 0.00009 -0.00037 2.59249

R25 2.59919 0.00029 0.00073 0.00036 0.00120 2.60038

R26 2.04117 -0.00013 -0.00039 0.00008 -0.00031 2.04086

R27 2.71707 -0.00043 -0.00052 -0.00098 -0.00147 2.71560

R28 2.04114 -0.00011 -0.00040 0.00019 -0.00021 2.04093

R29 2.59293 0.00005 -0.00036 0.00008 -0.00035 2.59258

R30 2.70448 -0.00002 0.00070 -0.00253 -0.00183 2.70266

R31 2.61601 0.00101 0.00179 0.00042 0.00221 2.61822

R32 2.81921 0.00012 0.00080 0.00109 0.00189 2.82110

R33 2.72993 -0.00084 -0.00075 -0.00219 -0.00290 2.72702

R34 2.62066 -0.00078 -0.00109 -0.00168 -0.00286 2.61780

R35 2.57102 0.00074 0.00025 0.00246 0.00281 2.57383

R36 2.03853 -0.00007 -0.00004 0.00007 0.00003 2.03855

R37 2.72993 -0.00084 -0.00075 -0.00219 -0.00290 2.72702

R38 2.03853 -0.00007 -0.00004 0.00007 0.00003 2.03855

R39 2.62066 -0.00078 -0.00109 -0.00168 -0.00286 2.61780

R40 2.61601 0.00101 0.00179 0.00042 0.00221 2.61822

R41 1.90994 0.00000 0.00000 0.00007 0.00007 1.91001

R42 2.81921 0.00012 0.00080 0.00109 0.00189 2.82110

R43 2.64735 -0.00012 -0.00109 -0.00045 -0.00154 2.64581

R44 2.64935 -0.00004 -0.00083 -0.00017 -0.00100 2.64835

R45 2.63382 0.00010 0.00022 0.00054 0.00077 2.63459

R46 2.05013 -0.00009 0.00007 -0.00027 -0.00020 2.04993

R47 2.63394 -0.00007 -0.00010 -0.00021 -0.00032 2.63362

R48 2.05095 -0.00002 -0.00016 0.00003 -0.00012 2.05082

R49 2.63660 -0.00005 -0.00008 -0.00012 -0.00020 2.63640

R50 2.05043 0.00001 -0.00004 0.00009 0.00005 2.05048

R51 2.63073 0.00011 0.00030 0.00068 0.00098 2.63171

R52 2.05095 -0.00003 -0.00015 0.00002 -0.00013 2.05083

R53 2.04985 -0.00010 -0.00000 -0.00027 -0.00027 2.04958

R54 2.63394 -0.00007 -0.00010 -0.00021 -0.00032 2.63362

R55 2.63660 -0.00005 -0.00008 -0.00012 -0.00020 2.63640

R56 2.05043 0.00001 -0.00004 0.00009 0.00005 2.05048

R57 2.63382 0.00010 0.00022 0.00054 0.00077 2.63459

R58 2.05095 -0.00002 -0.00016 0.00003 -0.00012 2.05082

R59 2.64735 -0.00012 -0.00109 -0.00045 -0.00154 2.64581

R60 2.05013 -0.00009 0.00007 -0.00027 -0.00020 2.04993

R61 2.64935 -0.00004 -0.00083 -0.00017 -0.00100 2.64835

R62 2.63073 0.00011 0.00030 0.00068 0.00098 2.63171

R63 2.04985 -0.00010 -0.00000 -0.00027 -0.00027 2.04958

R64 2.05095 -0.00003 -0.00015 0.00002 -0.00013 2.05083

R65 2.64948 -0.00009 -0.00091 -0.00037 -0.00128 2.64820

R66 2.64746 -0.00017 -0.00115 -0.00064 -0.00179 2.64567

R67 2.63068 0.00013 0.00032 0.00072 0.00105 2.63173

R68 2.04982 -0.00009 0.00001 -0.00020 -0.00018 2.04964

R69 2.63660 -0.00005 -0.00011 -0.00009 -0.00020 2.63640

R70 2.05096 -0.00003 -0.00015 0.00002 -0.00013 2.05083

R71 2.63393 -0.00007 -0.00008 -0.00021 -0.00029 2.63365

R72 2.05043 0.00001 -0.00004 0.00009 0.00005 2.05048

R73 2.63378 0.00011 0.00023 0.00060 0.00082 2.63461

R74 2.05095 -0.00002 -0.00016 0.00003 -0.00013 2.05082

R75 2.05010 -0.00007 0.00008 -0.00021 -0.00013 2.04997

R76 2.64948 -0.00009 -0.00091 -0.00037 -0.00128 2.64820

R77 2.64746 -0.00017 -0.00115 -0.00064 -0.00179 2.64567

R78 2.63068 0.00013 0.00032 0.00072 0.00105 2.63173

R79 2.04982 -0.00009 0.00001 -0.00020 -0.00018 2.04964

R80 2.63660 -0.00005 -0.00011 -0.00009 -0.00020 2.63640

R81 2.05096 -0.00003 -0.00015 0.00002 -0.00013 2.05083

R82 2.63393 -0.00007 -0.00008 -0.00021 -0.00029 2.63365

R83 2.05043 0.00001 -0.00004 0.00009 0.00005 2.05048

R84 2.63378 0.00011 0.00023 0.00060 0.00082 2.63461

R85 2.05095 -0.00002 -0.00016 0.00003 -0.00013 2.05082

R86 2.05010 -0.00007 0.00008 -0.00021 -0.00013 2.04997

A1 1.89722 -0.00028 -0.00020 -0.00114 -0.00136 1.89585

A2 2.17326 0.00012 -0.00082 0.00044 -0.00037 2.17289

A3 2.21261 0.00016 0.00107 0.00070 0.00177 2.21439

A4 1.84581 0.00028 -0.00000 0.00195 0.00192 1.84773

A5 2.22039 -0.00027 -0.00059 -0.00207 -0.00242 2.21796

A6 2.21696 -0.00001 0.00059 0.00011 0.00039 2.21736

A7 1.93870 -0.00000 0.00039 -0.00159 -0.00110 1.93760

A8 2.17014 0.00000 -0.00025 0.00101 0.00071 2.17084

A9 2.17014 0.00000 -0.00025 0.00101 0.00071 2.17084

A10 1.84581 0.00028 -0.00000 0.00195 0.00192 1.84773

A11 2.21696 -0.00001 0.00059 0.00011 0.00039 2.21736

A12 2.22039 -0.00027 -0.00059 -0.00207 -0.00242 2.21796

A13 1.89722 -0.00028 -0.00020 -0.00114 -0.00136 1.89585

A14 2.21261 0.00016 0.00107 0.00070 0.00177 2.21439

A15 2.17326 0.00012 -0.00082 0.00044 -0.00037 2.17289

A16 2.19040 0.00025 0.00325 0.00063 0.00350 2.19390

A17 2.04593 -0.00038 -0.00221 -0.00115 -0.00318 2.04274

A18 2.04685 0.00013 -0.00103 0.00054 -0.00031 2.04654

A19 2.19390 -0.00027 0.00044 -0.00194 -0.00184 2.19207

A20 2.15954 0.00027 0.00089 -0.00013 0.00100 2.16054

A21 1.92973 -0.00000 -0.00122 0.00209 0.00082 1.93056

A22 1.84883 -0.00003 0.00176 -0.00288 -0.00099 1.84784

A23 1.92963 0.00004 -0.00120 0.00232 0.00108 1.93071

A24 2.19384 -0.00025 0.00036 -0.00165 -0.00164 2.19219

A25 2.15971 0.00021 0.00096 -0.00065 0.00054 2.16025

A26 1.85825 -0.00002 0.00030 -0.00089 -0.00060 1.85765

A27 2.20329 0.00003 -0.00048 0.00058 0.00010 2.20340

A28 2.22151 -0.00001 0.00018 0.00037 0.00055 2.22206

A29 1.85820 0.00000 0.00037 -0.00074 -0.00038 1.85782

A30 2.20324 0.00003 -0.00057 0.00071 0.00015 2.20339

A31 2.22163 -0.00004 0.00020 0.00007 0.00027 2.22190

A32 2.19040 0.00025 0.00325 0.00063 0.00350 2.19390

A33 2.04593 -0.00038 -0.00221 -0.00115 -0.00318 2.04274

A34 2.04685 0.00013 -0.00103 0.00054 -0.00031 2.04654

A35 2.15954 0.00027 0.00089 -0.00013 0.00100 2.16054

A36 2.19390 -0.00027 0.00044 -0.00194 -0.00184 2.19207

A37 1.92973 -0.00000 -0.00122 0.00209 0.00082 1.93056

A38 1.85820 0.00000 0.00037 -0.00074 -0.00038 1.85782

A39 2.20324 0.00003 -0.00057 0.00071 0.00015 2.20339

A40 2.22163 -0.00004 0.00020 0.00007 0.00027 2.22190

A41 1.85825 -0.00002 0.00030 -0.00089 -0.00060 1.85765

A42 2.22151 -0.00001 0.00018 0.00037 0.00055 2.22206

A43 2.20329 0.00003 -0.00048 0.00058 0.00010 2.20340

A44 1.92963 0.00004 -0.00120 0.00232 0.00108 1.93071

A45 2.15971 0.00021 0.00096 -0.00065 0.00054 2.16025

A46 2.19384 -0.00025 0.00036 -0.00165 -0.00164 2.19219

A47 1.84883 -0.00003 0.00176 -0.00288 -0.00099 1.84784

A48 2.19028 0.00028 0.00334 0.00087 0.00381 2.19409

A49 2.04704 0.00011 -0.00122 0.00031 -0.00072 2.04632

A50 2.04584 -0.00039 -0.00211 -0.00116 -0.00307 2.04277

A51 2.22038 -0.00029 -0.00063 -0.00208 -0.00243 2.21795

A52 2.21712 -0.00003 0.00057 -0.00015 0.00009 2.21721

A53 1.84566 0.00032 0.00004 0.00223 0.00225 1.84790

A54 1.89725 -0.00030 -0.00021 -0.00128 -0.00151 1.89574

A55 2.17334 0.00011 -0.00075 0.00031 -0.00043 2.17291

A56 2.21248 0.00019 0.00101 0.00098 0.00200 2.21448

A57 1.89725 -0.00030 -0.00021 -0.00128 -0.00151 1.89574

A58 2.21248 0.00019 0.00101 0.00098 0.00200 2.21448

A59 2.17334 0.00011 -0.00075 0.00031 -0.00043 2.17291

A60 1.84566 0.00032 0.00004 0.00223 0.00225 1.84790

A61 2.22038 -0.00029 -0.00063 -0.00208 -0.00243 2.21795

A62 2.21712 -0.00003 0.00057 -0.00015 0.00009 2.21721

A63 1.93894 -0.00004 0.00033 -0.00187 -0.00145 1.93749

A64 2.17043 0.00002 -0.00037 0.00104 0.00061 2.17103

A65 2.17043 0.00002 -0.00037 0.00104 0.00061 2.17103

A66 2.19028 0.00028 0.00334 0.00087 0.00381 2.19409

A67 2.04704 0.00011 -0.00122 0.00031 -0.00072 2.04632

A68 2.04584 -0.00039 -0.00211 -0.00116 -0.00307 2.04277

A69 2.11578 -0.00025 -0.00126 -0.00156 -0.00282 2.11296

A70 2.10342 -0.00005 -0.00112 0.00035 -0.00078 2.10264

A71 2.06398 0.00030 0.00239 0.00121 0.00360 2.06758

A72 2.11060 -0.00018 -0.00133 -0.00068 -0.00201 2.10859

A73 2.08164 0.00006 0.00075 -0.00032 0.00043 2.08207

A74 2.09092 0.00012 0.00058 0.00101 0.00159 2.09251

A75 2.09775 -0.00001 -0.00014 -0.00014 -0.00028 2.09747

A76 2.08848 0.00005 0.00003 0.00063 0.00066 2.08914

A77 2.09694 -0.00003 0.00013 -0.00050 -0.00037 2.09657

A78 2.08534 0.00012 0.00066 0.00057 0.00124 2.08658

A79 2.09906 -0.00006 -0.00033 -0.00026 -0.00058 2.09848

A80 2.09878 -0.00006 -0.00034 -0.00032 -0.00065 2.09813

A81 2.09774 -0.00002 -0.00018 -0.00019 -0.00038 2.09736

A82 2.09648 -0.00003 0.00014 -0.00050 -0.00036 2.09612

A83 2.08895 0.00005 0.00005 0.00070 0.00074 2.08970

A84 2.11093 -0.00020 -0.00139 -0.00077 -0.00216 2.10877

A85 2.08130 0.00007 0.00078 -0.00020 0.00058 2.08188

A86 2.09092 0.00013 0.00061 0.00097 0.00158 2.09251

A87 2.08534 0.00012 0.00066 0.00057 0.00124 2.08658

A88 2.09906 -0.00006 -0.00033 -0.00026 -0.00058 2.09848

A89 2.09878 -0.00006 -0.00034 -0.00032 -0.00065 2.09813

A90 2.09775 -0.00001 -0.00014 -0.00014 -0.00028 2.09747

A91 2.09694 -0.00003 0.00013 -0.00050 -0.00037 2.09657

A92 2.08848 0.00005 0.00003 0.00063 0.00066 2.08914

A93 2.11060 -0.00018 -0.00133 -0.00068 -0.00201 2.10859

A94 2.09092 0.00012 0.00058 0.00101 0.00159 2.09251

A95 2.08164 0.00006 0.00075 -0.00032 0.00043 2.08207

A96 2.11578 -0.00025 -0.00126 -0.00156 -0.00282 2.11296

A97 2.10342 -0.00005 -0.00112 0.00035 -0.00078 2.10264

A98 2.06398 0.00030 0.00239 0.00121 0.00360 2.06758

A99 2.11093 -0.00020 -0.00139 -0.00077 -0.00216 2.10877

A100 2.08130 0.00007 0.00078 -0.00020 0.00058 2.08188

A101 2.09092 0.00013 0.00061 0.00097 0.00158 2.09251

A102 2.09774 -0.00002 -0.00018 -0.00019 -0.00038 2.09736

A103 2.09648 -0.00003 0.00014 -0.00050 -0.00036 2.09612

A104 2.08895 0.00005 0.00005 0.00070 0.00074 2.08970

A105 2.10355 -0.00008 -0.00115 0.00007 -0.00108 2.10247

A106 2.11587 -0.00027 -0.00131 -0.00163 -0.00295 2.11292

A107 2.06376 0.00035 0.00247 0.00156 0.00403 2.06779

A108 2.11103 -0.00022 -0.00141 -0.00094 -0.00235 2.10869

A109 2.08129 0.00008 0.00078 -0.00019 0.00059 2.08188

A110 2.09082 0.00015 0.00063 0.00113 0.00176 2.09259

A111 2.09779 -0.00003 -0.00021 -0.00026 -0.00047 2.09732

A112 2.08890 0.00006 0.00005 0.00074 0.00080 2.08970

A113 2.09649 -0.00003 0.00016 -0.00049 -0.00033 2.09616

A114 2.08526 0.00013 0.00068 0.00068 0.00136 2.08662

A115 2.09882 -0.00007 -0.00035 -0.00037 -0.00072 2.09810

A116 2.09911 -0.00006 -0.00033 -0.00032 -0.00065 2.09846

A117 2.09780 -0.00003 -0.00015 -0.00020 -0.00035 2.09745

A118 2.09695 -0.00003 0.00014 -0.00050 -0.00036 2.09659

A119 2.08842 0.00006 0.00002 0.00070 0.00072 2.08914

A120 2.11070 -0.00020 -0.00137 -0.00085 -0.00222 2.10848

A121 2.08163 0.00006 0.00076 -0.00032 0.00044 2.08207

A122 2.09082 0.00014 0.00062 0.00119 0.00181 2.09263

A123 2.10355 -0.00008 -0.00115 0.00007 -0.00108 2.10247

A124 2.11587 -0.00027 -0.00131 -0.00163 -0.00295 2.11292

A125 2.06376 0.00035 0.00247 0.00156 0.00403 2.06779

A126 2.11103 -0.00022 -0.00141 -0.00094 -0.00235 2.10869

A127 2.08129 0.00008 0.00078 -0.00019 0.00059 2.08188

A128 2.09082 0.00015 0.00063 0.00113 0.00176 2.09259

A129 2.09779 -0.00003 -0.00021 -0.00026 -0.00047 2.09732

A130 2.08890 0.00006 0.00005 0.00074 0.00080 2.08970

A131 2.09649 -0.00003 0.00016 -0.00049 -0.00033 2.09616

A132 2.08526 0.00013 0.00068 0.00068 0.00136 2.08662

A133 2.09882 -0.00007 -0.00035 -0.00037 -0.00072 2.09810

A134 2.09911 -0.00006 -0.00033 -0.00032 -0.00065 2.09846

A135 2.09780 -0.00003 -0.00015 -0.00020 -0.00035 2.09745

A136 2.09695 -0.00003 0.00014 -0.00050 -0.00036 2.09659

A137 2.08842 0.00006 0.00002 0.00070 0.00072 2.08914

A138 2.11070 -0.00020 -0.00137 -0.00085 -0.00222 2.10848

A139 2.08163 0.00006 0.00076 -0.00032 0.00044 2.08207

A140 2.09082 0.00014 0.00062 0.00119 0.00181 2.09263

D1 0.00289 0.00000 -0.00113 -0.00303 -0.00416 -0.00127

D2 3.13762 -0.00010 -0.00963 -0.00432 -0.01395 3.12368

D3 -3.12488 0.00002 -0.00465 -0.00240 -0.00704 -3.13192

D4 0.00986 -0.00008 -0.01315 -0.00369 -0.01683 -0.00696

D5 -0.00000 0.00000 -0.00000 -0.00000 -0.00000 -0.00000

D6 -3.12737 0.00002 -0.00359 0.00065 -0.00294 -3.13031

D7 3.12737 -0.00002 0.00359 -0.00065 0.00294 3.13031

D8 0.00000 -0.00000 0.00000 0.00000 -0.00000 0.00000

D9 -0.00483 -0.00000 0.00189 0.00507 0.00696 0.00213

D10 3.04188 0.00007 0.00070 0.00983 0.01052 3.05241

D11 -3.13959 0.00010 0.01036 0.00637 0.01676 -3.12283

D12 -0.09287 0.00017 0.00917 0.01113 0.02032 -0.07255

D13 -3.08403 0.00011 -0.00062 -0.00135 -0.00198 -3.08601

D14 0.05179 0.00013 0.00042 0.00130 0.00172 0.05352

D15 0.04930 -0.00002 -0.01086 -0.00291 -0.01377 0.03553

D16 -3.09806 0.00000 -0.00981 -0.00026 -0.01007 -3.10813

D17 0.00483 0.00000 -0.00189 -0.00507 -0.00696 -0.00213

D18 3.13959 -0.00010 -0.01036 -0.00637 -0.01676 3.12283

D19 -3.04188 -0.00007 -0.00070 -0.00983 -0.01052 -3.05241

D20 0.09287 -0.00017 -0.00917 -0.01113 -0.02032 0.07255

D21 -0.00289 -0.00000 0.00113 0.00303 0.00416 0.00127

D22 3.12488 -0.00002 0.00465 0.00240 0.00704 3.13192

D23 -3.13762 0.00010 0.00963 0.00432 0.01395 -3.12368

D24 -0.00986 0.00008 0.01315 0.00369 0.01683 0.00696

D25 -0.04930 0.00002 0.01086 0.00291 0.01377 -0.03553

D26 3.09806 -0.00000 0.00981 0.00026 0.01007 3.10813

D27 3.08403 -0.00011 0.00062 0.00135 0.00198 3.08601

D28 -0.05179 -0.00013 -0.00042 -0.00130 -0.00172 -0.05352

D29 -0.13280 0.00018 0.02036 0.01645 0.03682 -0.09598

D30 3.01346 -0.00003 0.01234 0.01140 0.02374 3.03720

D31 3.00302 0.00020 0.02141 0.01909 0.04052 3.04354

D32 -0.13390 -0.00001 0.01339 0.01405 0.02744 -0.10647

D33 -1.10381 -0.00018 -0.02906 -0.00672 -0.03579 -1.13959

D34 2.03967 -0.00020 -0.03155 -0.00562 -0.03718 2.00249

D35 2.04307 -0.00020 -0.03004 -0.00915 -0.03918 2.00389

D36 -1.09664 -0.00022 -0.03253 -0.00805 -0.04057 -1.13721

D37 -3.12203 0.00006 -0.00937 0.00125 -0.00814 -3.13018

D38 0.01541 0.00024 -0.00224 0.00572 0.00347 0.01888

D39 3.12764 0.00004 0.00828 0.00120 0.00948 3.13712

D40 -0.02943 0.00007 0.00857 0.00365 0.01222 -0.01721

D41 -0.00991 -0.00014 0.00130 -0.00317 -0.00187 -0.01178

D42 3.11621 -0.00011 0.00159 -0.00072 0.00087 3.11708

D43 -0.01519 -0.00025 0.00237 -0.00616 -0.00378 -0.01897

D44 3.12197 -0.00005 0.00966 -0.00098 0.00870 3.13067

D45 0.00931 0.00017 -0.00163 0.00433 0.00269 0.01201

D46 -3.11611 0.00012 -0.00166 0.00078 -0.00088 -3.11699

D47 -3.12795 -0.00002 -0.00877 -0.00073 -0.00951 -3.13746

D48 0.02981 -0.00007 -0.00880 -0.00428 -0.01309 0.01673

D49 0.13242 -0.00018 -0.02063 -0.01634 -0.03698 0.09544

D50 -3.00277 -0.00022 -0.02100 -0.02051 -0.04152 -3.04429

D51 -3.01417 0.00004 -0.01243 -0.01050 -0.02293 -3.03709

D52 0.13383 0.00000 -0.01280 -0.01467 -0.02747 0.10636

D53 0.00035 -0.00002 0.00020 -0.00067 -0.00048 -0.00013

D54 -3.12556 -0.00005 -0.00009 -0.00316 -0.00325 -3.12881

D55 3.12555 0.00004 0.00022 0.00293 0.00315 3.12869

D56 -0.00036 0.00001 -0.00007 0.00044 0.00037 0.00001

D57 -3.01346 0.00003 -0.01234 -0.01140 -0.02374 -3.03720

D58 0.13280 -0.00018 -0.02036 -0.01645 -0.03682 0.09598

D59 0.13390 0.00001 -0.01339 -0.01405 -0.02744 0.10647

D60 -3.00302 -0.00020 -0.02141 -0.01909 -0.04052 -3.04354

D61 1.10381 0.00018 0.02906 0.00672 0.03579 1.13959

D62 -2.03967 0.00020 0.03155 0.00562 0.03718 -2.00249

D63 -2.04307 0.00020 0.03004 0.00915 0.03918 -2.00389

D64 1.09664 0.00022 0.03253 0.00805 0.04057 1.13721

D65 -3.12764 -0.00004 -0.00828 -0.00120 -0.00948 -3.13712

D66 0.02943 -0.00007 -0.00857 -0.00365 -0.01222 0.01721

D67 0.00991 0.00014 -0.00130 0.00317 0.00187 0.01178

D68 -3.11621 0.00011 -0.00159 0.00072 -0.00087 -3.11708

D69 3.12203 -0.00006 0.00937 -0.00125 0.00814 3.13018

D70 -0.01541 -0.00024 0.00224 -0.00572 -0.00347 -0.01888

D71 -0.00035 0.00002 -0.00020 0.00067 0.00048 0.00013

D72 -3.12555 -0.00004 -0.00022 -0.00293 -0.00315 -3.12869

D73 3.12556 0.00005 0.00009 0.00316 0.00325 3.12881

D74 0.00036 -0.00001 0.00007 -0.00044 -0.00037 -0.00001

D75 -0.00931 -0.00017 0.00163 -0.00433 -0.00269 -0.01201

D76 3.12795 0.00002 0.00877 0.00073 0.00951 3.13746

D77 3.11611 -0.00012 0.00166 -0.00078 0.00088 3.11699

D78 -0.02981 0.00007 0.00880 0.00428 0.01309 -0.01673

D79 0.01519 0.00025 -0.00237 0.00616 0.00378 0.01897

D80 -3.12197 0.00005 -0.00966 0.00098 -0.00870 -3.13067

D81 3.01417 -0.00004 0.01243 0.01050 0.02293 3.03709

D82 -0.13383 -0.00000 0.01280 0.01467 0.02747 -0.10636

D83 -0.13242 0.00018 0.02063 0.01634 0.03698 -0.09544

D84 3.00277 0.00022 0.02100 0.02051 0.04152 3.04429

D85 3.08256 -0.00007 0.00206 0.00347 0.00552 3.08808

D86 -0.04989 0.00004 0.01059 0.00528 0.01587 -0.03402

D87 -0.05263 -0.00011 0.00169 -0.00070 0.00098 -0.05165

D88 3.09810 0.00000 0.01022 0.00111 0.01133 3.10944

D89 -1.09669 -0.00021 -0.03688 -0.00611 -0.04298 -1.13967

D90 2.04323 -0.00019 -0.03462 -0.00731 -0.04192 2.00131

D91 2.03904 -0.00017 -0.03652 -0.00229 -0.03882 2.00022

D92 -1.10423 -0.00015 -0.03426 -0.00348 -0.03775 -1.14198

D93 -3.13757 0.00009 0.00912 0.00394 0.01306 -3.12451

D94 -0.01111 0.00009 0.01260 0.00487 0.01746 0.00636

D95 -0.00356 -0.00001 0.00204 0.00243 0.00447 0.00091

D96 3.12290 -0.00001 0.00552 0.00336 0.00887 3.13177

D97 3.13999 -0.00008 -0.01046 -0.00559 -0.01608 3.12391

D98 0.08363 -0.00013 -0.00499 -0.00816 -0.01317 0.07047

D99 0.00596 0.00001 -0.00340 -0.00408 -0.00748 -0.00152

D100 -3.05039 -0.00003 0.00207 -0.00665 -0.00457 -3.05496

D101 0.00000 0.00000 -0.00000 -0.00000 0.00000 0.00000

D102 3.12603 -0.00000 0.00356 0.00095 0.00451 3.13054

D103 -3.12603 0.00000 -0.00356 -0.00095 -0.00451 -3.13054

D104 -0.00000 -0.00000 -0.00000 0.00000 -0.00000 -0.00000

D105 0.00356 0.00001 -0.00204 -0.00243 -0.00447 -0.00091

D106 3.13757 -0.00009 -0.00912 -0.00394 -0.01306 3.12451

D107 -3.12290 0.00001 -0.00552 -0.00336 -0.00887 -3.13177

D108 0.01111 -0.00009 -0.01260 -0.00487 -0.01746 -0.00636

D109 -0.00596 -0.00001 0.00340 0.00408 0.00748 0.00152

D110 3.05039 0.00003 -0.00207 0.00665 0.00457 3.05496

D111 -3.13999 0.00008 0.01046 0.00559 0.01608 -3.12391

D112 -0.08363 0.00013 0.00499 0.00816 0.01317 -0.07047

D113 -3.08256 0.00007 -0.00206 -0.00347 -0.00552 -3.08808

D114 0.05263 0.00011 -0.00169 0.00070 -0.00098 0.05165

D115 0.04989 -0.00004 -0.01059 -0.00528 -0.01587 0.03402

D116 -3.09810 -0.00000 -0.01022 -0.00111 -0.01133 -3.10944

D117 1.09669 0.00021 0.03688 0.00611 0.04298 1.13967

D118 -2.04323 0.00019 0.03462 0.00731 0.04192 -2.00131

D119 -2.03904 0.00017 0.03652 0.00229 0.03882 -2.00022

D120 1.10423 0.00015 0.03426 0.00348 0.03775 1.14198

D121 3.13628 0.00002 -0.00060 0.00129 0.00069 3.13697

D122 -0.01326 -0.00001 0.00083 0.00259 0.00342 -0.00984

D123 -0.00715 0.00004 0.00183 0.00022 0.00205 -0.00510

D124 3.12649 0.00001 0.00326 0.00152 0.00478 3.13127

D125 -3.13652 0.00004 0.00223 -0.00050 0.00173 -3.13480

D126 -0.00403 0.00000 0.00280 0.00002 0.00282 -0.00121

D127 0.00689 0.00001 -0.00018 0.00056 0.00038 0.00727

D128 3.13938 -0.00002 0.00039 0.00109 0.00147 3.14086

D129 0.00354 -0.00006 -0.00220 -0.00054 -0.00275 0.00079

D130 3.13969 -0.00005 -0.00031 -0.00111 -0.00142 3.13827

D131 -3.13006 -0.00003 -0.00364 -0.00185 -0.00549 -3.13554

D132 0.00609 -0.00002 -0.00174 -0.00242 -0.00416 0.00193

D133 0.00051 0.00002 0.00087 0.00008 0.00095 0.00147

D134 3.14092 0.00003 0.00122 0.00042 0.00164 -3.14063

D135 -3.13561 0.00001 -0.00103 0.00065 -0.00038 -3.13599

D136 0.00480 0.00001 -0.00069 0.00099 0.00030 0.00510

D137 -0.00077 0.00003 0.00076 0.00069 0.00146 0.00069

D138 -3.13817 0.00002 -0.00011 0.00115 0.00104 -3.13713

D139 -3.14118 0.00003 0.00041 0.00035 0.00077 -3.14041

D140 0.00461 0.00002 -0.00045 0.00081 0.00036 0.00497

D141 -0.00302 -0.00005 -0.00110 -0.00102 -0.00212 -0.00514

D142 -3.13546 -0.00002 -0.00168 -0.00154 -0.00322 -3.13868

D143 3.13440 -0.00004 -0.00024 -0.00148 -0.00171 3.13268

D144 0.00196 -0.00001 -0.00081 -0.00200 -0.00281 -0.00086

D145 -0.00051 -0.00002 -0.00087 -0.00008 -0.00095 -0.00147

D146 3.13561 -0.00001 0.00103 -0.00065 0.00038 3.13599

D147 -3.14092 -0.00003 -0.00122 -0.00042 -0.00164 3.14063

D148 -0.00480 -0.00001 0.00069 -0.00099 -0.00030 -0.00510

D149 0.00077 -0.00003 -0.00076 -0.00069 -0.00146 -0.00069

D150 3.13817 -0.00002 0.00011 -0.00115 -0.00104 3.13713

D151 3.14118 -0.00003 -0.00041 -0.00035 -0.00077 3.14041

D152 -0.00461 -0.00002 0.00045 -0.00081 -0.00036 -0.00497

D153 -0.00354 0.00006 0.00220 0.00054 0.00275 -0.00079

D154 3.13006 0.00003 0.00364 0.00185 0.00549 3.13554

D155 -3.13969 0.00005 0.00031 0.00111 0.00142 -3.13827

D156 -0.00609 0.00002 0.00174 0.00242 0.00416 -0.00193

D157 -3.13628 -0.00002 0.00060 -0.00129 -0.00069 -3.13697

D158 0.00715 -0.00004 -0.00183 -0.00022 -0.00205 0.00510

D159 0.01326 0.00001 -0.00083 -0.00259 -0.00342 0.00984

D160 -3.12649 -0.00001 -0.00326 -0.00152 -0.00478 -3.13127

D161 3.13652 -0.00004 -0.00223 0.00050 -0.00173 3.13480

D162 0.00403 -0.00000 -0.00280 -0.00002 -0.00282 0.00121

D163 -0.00689 -0.00001 0.00018 -0.00056 -0.00038 -0.00727

D164 -3.13938 0.00002 -0.00039 -0.00109 -0.00147 -3.14086

D165 0.00302 0.00005 0.00110 0.00102 0.00212 0.00514

D166 -3.13440 0.00004 0.00024 0.00148 0.00171 -3.13268

D167 3.13546 0.00002 0.00168 0.00154 0.00322 3.13868

D168 -0.00196 0.00001 0.00081 0.00200 0.00281 0.00086

D169 3.13621 -0.00003 -0.00178 0.00049 -0.00130 3.13491

D170 0.00404 -0.00001 -0.00234 -0.00050 -0.00284 0.00120

D171 -0.00701 -0.00001 0.00040 -0.00067 -0.00027 -0.00728

D172 -3.13917 0.00001 -0.00015 -0.00166 -0.00181 -3.14098

D173 -3.13604 -0.00002 -0.00005 -0.00118 -0.00123 -3.13727

D174 0.01388 -0.00000 -0.00124 -0.00347 -0.00471 0.00917

D175 0.00719 -0.00004 -0.00225 -0.00002 -0.00227 0.00492

D176 -3.12608 -0.00002 -0.00344 -0.00231 -0.00575 -3.13183

D177 0.00312 0.00005 0.00116 0.00105 0.00221 0.00534

D178 -3.13428 0.00004 0.00023 0.00136 0.00160 -3.13269

D179 3.13524 0.00002 0.00171 0.00204 0.00376 3.13900

D180 -0.00217 0.00001 0.00079 0.00235 0.00314 0.00097

D181 0.00076 -0.00003 -0.00091 -0.00074 -0.00164 -0.00088

D182 3.14119 -0.00003 -0.00050 -0.00036 -0.00086 3.14032

D183 3.13815 -0.00002 0.00002 -0.00105 -0.00103 3.13713

D184 -0.00461 -0.00001 0.00043 -0.00067 -0.00024 -0.00485

D185 -0.00058 -0.00002 -0.00092 0.00005 -0.00087 -0.00146

D186 3.13555 -0.00000 0.00112 -0.00041 0.00070 3.13625

D187 -3.14101 -0.00003 -0.00133 -0.00032 -0.00165 3.14052

D188 -0.00488 -0.00001 0.00071 -0.00079 -0.00008 -0.00496

D189 -0.00348 0.00006 0.00255 0.00033 0.00287 -0.00061

D190 3.12974 0.00004 0.00375 0.00262 0.00637 3.13611

D191 -3.13964 0.00004 0.00051 0.00080 0.00131 -3.13834

D192 -0.00642 0.00002 0.00171 0.00309 0.00480 -0.00162

D193 -3.13621 0.00003 0.00178 -0.00049 0.00130 -3.13491

D194 -0.00404 0.00001 0.00234 0.00050 0.00284 -0.00120

D195 0.00701 0.00001 -0.00040 0.00067 0.00027 0.00728

D196 3.13917 -0.00001 0.00015 0.00166 0.00181 3.14098

D197 3.13604 0.00002 0.00005 0.00118 0.00123 3.13727

D198 -0.01388 0.00000 0.00124 0.00347 0.00471 -0.00917

D199 -0.00719 0.00004 0.00225 0.00002 0.00227 -0.00492

D200 3.12608 0.00002 0.00344 0.00231 0.00575 3.13183

D201 -0.00312 -0.00005 -0.00116 -0.00105 -0.00221 -0.00534

D202 3.13428 -0.00004 -0.00023 -0.00136 -0.00160 3.13269

D203 -3.13524 -0.00002 -0.00171 -0.00204 -0.00376 -3.13900

D204 0.00217 -0.00001 -0.00079 -0.00235 -0.00314 -0.00097

D205 -0.00076 0.00003 0.00091 0.00074 0.00164 0.00088

D206 -3.14119 0.00003 0.00050 0.00036 0.00086 -3.14032

D207 -3.13815 0.00002 -0.00002 0.00105 0.00103 -3.13713

D208 0.00461 0.00001 -0.00043 0.00067 0.00024 0.00485

D209 0.00058 0.00002 0.00092 -0.00005 0.00087 0.00146

D210 -3.13555 0.00000 -0.00112 0.00041 -0.00070 -3.13625

D211 3.14101 0.00003 0.00133 0.00032 0.00165 -3.14052

D212 0.00488 0.00001 -0.00071 0.00079 0.00008 0.00496

D213 0.00348 -0.00006 -0.00255 -0.00033 -0.00287 0.00061

D214 -3.12974 -0.00004 -0.00375 -0.00262 -0.00637 -3.13611

D215 3.13964 -0.00004 -0.00051 -0.00080 -0.00131 3.13834

D216 0.00642 -0.00002 -0.00171 -0.00309 -0.00480 0.00162

Item Value Threshold Converged?

Maximum Force 0.001169 0.000450 NO

RMS Force 0.000201 0.000300 YES

Maximum Displacement 0.233142 0.001800 NO

RMS Displacement 0.063893 0.001200 NO

Predicted change in Energy=-1.239659D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Aug 18 14:29:30 2019, MaxMem= 2013265920 cpu: 1.6

(Enter /home/kira/g09/l202.exe)

Stoichiometry C44H30N4(1-,2)

Framework group CS[SG(H2N2),X(C44H28N2)]

Deg. of freedom 116

Full point group CS NOp 2

RotChk: IX=3 Diff= 1.49D-04

Largest Abelian subgroup CS NOp 2

Largest concise Abelian subgroup CS NOp 2

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 4.261697 -0.094075 0.680981

2 6 0 2.898796 0.018183 1.141848

3 7 0 2.117054 0.084276 0.000000

4 6 0 2.898796 0.018183 -1.141848

5 6 0 4.261697 -0.094075 -0.680981

6 6 0 2.459935 0.034460 -2.456086

7 6 0 1.094580 0.082781 -2.879623

8 7 0 -0.000041 0.013808 -2.055536

9 6 0 -1.094908 0.082251 -2.879420

10 6 0 -0.688491 0.222289 -4.250652

11 6 0 0.687572 0.222509 -4.250798

12 6 0 2.459935 0.034460 2.456086

13 6 0 1.094580 0.082781 2.879623

14 6 0 0.687572 0.222509 4.250798

15 6 0 -0.688491 0.222289 4.250652

16 6 0 -1.094908 0.082251 2.879420

17 7 0 -0.000041 0.013808 2.055536

18 6 0 -2.460047 0.033859 2.455767

19 6 0 -2.898934 0.017398 1.141716

20 6 0 -4.262067 -0.092568 0.681007

21 6 0 -4.262067 -0.092568 -0.681007

22 6 0 -2.898934 0.017398 -1.141716

23 7 0 -2.117040 0.081689 -0.000000

24 6 0 -2.460047 0.033859 -2.455767

25 6 0 3.505254 -0.004406 -3.521214

26 6 0 4.408963 1.052298 -3.685448

27 6 0 5.386616 1.008093 -4.678389

28 6 0 5.475705 -0.095224 -5.525156

29 6 0 4.579217 -1.153342 -5.373280

30 6 0 3.601827 -1.105830 -4.382373

31 6 0 5.475705 -0.095224 5.525156

32 6 0 5.386616 1.008093 4.678389

33 6 0 4.408963 1.052298 3.685448

34 6 0 3.505254 -0.004406 3.521214

35 6 0 3.601827 -1.105830 4.382373

36 6 0 4.579217 -1.153342 5.373280

37 6 0 -3.505266 -0.004604 -3.520976

38 6 0 -3.603508 -1.107085 -4.380463

39 6 0 -4.580725 -1.154264 -5.371572

40 6 0 -5.475085 -0.094617 -5.525332

41 6 0 -5.384230 1.009776 -4.680129

42 6 0 -4.406890 1.053529 -3.686845

43 6 0 -3.505266 -0.004604 3.520976

44 6 0 -3.603508 -1.107085 4.380463

45 6 0 -4.580725 -1.154264 5.371572

46 6 0 -5.475085 -0.094617 5.525332

47 6 0 -5.384230 1.009776 4.680129

48 6 0 -4.406890 1.053529 3.686845

49 1 0 5.120852 -0.174608 1.328293

50 1 0 5.120852 -0.174608 -1.328293

51 1 0 -1.343294 0.320317 -5.103911

52 1 0 1.342001 0.320767 -5.104270

53 1 0 1.342001 0.320767 5.104270

54 1 0 -1.343294 0.320317 5.103911

55 1 0 -5.121339 -0.171455 1.328420

56 1 0 -5.121339 -0.171455 -1.328420

57 1 0 4.340193 1.915844 -3.032532

58 1 0 6.075883 1.838664 -4.791649

59 1 0 6.236812 -0.131008 -6.297691

60 1 0 4.643198 -2.018692 -6.025082

61 1 0 2.908923 -1.932149 -4.266549

62 1 0 6.236812 -0.131008 6.297691

63 1 0 6.075883 1.838664 4.791649

64 1 0 4.340193 1.915844 3.032532

65 1 0 2.908923 -1.932149 4.266549

66 1 0 4.643198 -2.018692 6.025082

67 1 0 -2.912001 -1.934420 -4.263257

68 1 0 -4.646098 -2.020441 -6.022138

69 1 0 -6.236002 -0.130096 -6.298065

70 1 0 -6.071994 1.841409 -4.794721

71 1 0 -4.336955 1.917621 -3.034740

72 1 0 -2.912001 -1.934420 4.263257

73 1 0 -4.646098 -2.020441 6.022138

74 1 0 -6.236002 -0.130096 6.298065

75 1 0 -6.071994 1.841409 4.794721

76 1 0 -4.336955 1.917621 3.034740

77 1 0 1.106337 0.093387 0.000000

78 1 0 -1.106349 0.091114 -0.000000

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

Rotational constants (GHZ): 0.0583443 0.0578303 0.0300415

Leave Link 202 at Sun Aug 18 14:29:30 2019, MaxMem= 2013265920 cpu: 0.1

(Enter /home/kira/g09/l301.exe)

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

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

There are 513 symmetry adapted cartesian basis functions of A' symmetry.

There are 489 symmetry adapted cartesian basis functions of A" symmetry.

There are 488 symmetry adapted basis functions of A' symmetry.

There are 466 symmetry adapted basis functions of A" symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 161 beta electrons

nuclear repulsion energy 5346.2402885713 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= 78 NActive= 78 NUniq= 41 SFac= 3.62D+00 NAtFMM= 60 NAOKFM=T 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= -0.2116293157 Hartrees.

Nuclear repulsion after empirical dispersion term = 5346.0286592555 Hartrees.

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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= 78.

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

Smoothing algorithm: York/Karplus (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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5788

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.26D-08

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 378

GePol: Fraction of low-weight points (<1% of avg) = 6.53%

GePol: Cavity surface area = 618.009 Ang\*\*2

GePol: Cavity volume = 629.823 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0019692969 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5346.0266899587 Hartrees.

Leave Link 301 at Sun Aug 18 14:29:30 2019, MaxMem= 2013265920 cpu: 1.1

(Enter /home/kira/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.

One-electron integral symmetry used in STVInt

NBasis= 954 RedAO= T EigKep= 8.95D-05 NBF= 488 466

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 488 466

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= 938 938 939 939 940 MxSgAt= 78 MxSgA2= 78.

Leave Link 302 at Sun Aug 18 14:29:32 2019, MaxMem= 2013265920 cpu: 11.1

(Enter /home/kira/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sun Aug 18 14:29:32 2019, MaxMem= 2013265920 cpu: 1.3

(Enter /home/kira/g09/l401.exe)

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

B after Tr= 0.000000 -0.000000 -0.000000

Rot= 1.000000 -0.000000 0.000000 0.000026 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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The electronic state of the initial guess is 2-A'.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7585 S= 0.5043

Generating alternative initial guess.

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2000

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= -1914.58014295361

Leave Link 401 at Sun Aug 18 14:29:38 2019, MaxMem= 2013265920 cpu: 49.6

(Enter /home/kira/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3047318 IEndB= 3047318 NGot= 2013265920 MDV= 2011240249

LenX= 2011240249 LenY= 2010235243

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= 480000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 100502832.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.22D-15 for 4495.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.34D-15 for 2415 1484.

Iteration 1 A^-1\*A deviation from unit magnitude is 8.22D-15 for 5766.

Iteration 1 A^-1\*A deviation from orthogonality is 7.52D-12 for 5785 5580.

E= -1914.46176694949

DIIS: error= 6.15D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.46176694949 IErMin= 1 ErrMin= 6.15D-03

ErrMax= 6.15D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.90D-02 BMatP= 5.90D-02

IDIUse=3 WtCom= 9.38D-01 WtEn= 6.15D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.446 Goal= None Shift= 0.000

Gap= 0.504 Goal= None Shift= 0.000

GapD= 0.446 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=1.71D-04 MaxDP=4.54D-03 OVMax= 3.01D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.71D-04 CP: 1.00D+00

E= -1914.49302629826 Delta-E= -0.031259348769 Rises=F Damp=F

DIIS: error= 8.23D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.49302629826 IErMin= 2 ErrMin= 8.23D-04

ErrMax= 8.23D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.08D-04 BMatP= 5.90D-02

IDIUse=3 WtCom= 9.92D-01 WtEn= 8.23D-03

Coeff-Com: -0.723D-01 0.107D+01

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

Coeff: -0.717D-01 0.107D+01

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=3.09D-05 MaxDP=7.66D-04 DE=-3.13D-02 OVMax= 4.63D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.72D-05 CP: 1.00D+00 1.09D+00

E= -1914.49353691940 Delta-E= -0.000510621135 Rises=F Damp=F

DIIS: error= 1.88D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.49353691940 IErMin= 3 ErrMin= 1.88D-04

ErrMax= 1.88D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.05D-04 BMatP= 8.08D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.88D-03

Coeff-Com: -0.237D-01 0.275D+00 0.749D+00

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

Coeff: -0.236D-01 0.274D+00 0.749D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=9.54D-06 MaxDP=5.73D-04 DE=-5.11D-04 OVMax= 1.86D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 8.35D-06 CP: 1.00D+00 1.10D+00 8.71D-01

E= -1914.49355000907 Delta-E= -0.000013089671 Rises=F Damp=F

DIIS: error= 1.99D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.49355000907 IErMin= 3 ErrMin= 1.88D-04

ErrMax= 1.99D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.43D-05 BMatP= 1.05D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.99D-03

Coeff-Com: -0.830D-02 0.776D-01 0.444D+00 0.487D+00

Coeff-En: 0.000D+00 0.000D+00 0.330D+00 0.670D+00

Coeff: -0.828D-02 0.774D-01 0.444D+00 0.487D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=4.58D-06 MaxDP=3.85D-04 DE=-1.31D-05 OVMax= 1.21D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.26D-06 CP: 1.00D+00 1.10D+00 9.10D-01 6.40D-01

E= -1914.49356426824 Delta-E= -0.000014259171 Rises=F Damp=F

DIIS: error= 4.45D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.49356426824 IErMin= 5 ErrMin= 4.45D-05

ErrMax= 4.45D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.48D-06 BMatP= 6.43D-05

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

Coeff-Com: 0.629D-03-0.191D-01 0.577D-01 0.230D+00 0.730D+00

Coeff: 0.629D-03-0.191D-01 0.577D-01 0.230D+00 0.730D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=1.48D-06 MaxDP=8.36D-05 DE=-1.43D-05 OVMax= 3.57D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 7.90D-07 CP: 1.00D+00 1.10D+00 9.31D-01 7.18D-01 7.22D-01

E= -1914.49356529420 Delta-E= -0.000001025966 Rises=F Damp=F

DIIS: error= 1.42D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.49356529420 IErMin= 6 ErrMin= 1.42D-05

ErrMax= 1.42D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.91D-07 BMatP= 4.48D-06

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

Coeff-Com: 0.764D-03-0.149D-01 0.100D-01 0.107D+00 0.420D+00 0.478D+00

Coeff: 0.764D-03-0.149D-01 0.100D-01 0.107D+00 0.420D+00 0.478D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=4.45D-07 MaxDP=2.08D-05 DE=-1.03D-06 OVMax= 9.51D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.33D-07 CP: 1.00D+00 1.10D+00 9.34D-01 7.15D-01 7.64D-01

CP: 5.75D-01

E= -1914.49356544659 Delta-E= -0.000000152384 Rises=F Damp=F

DIIS: error= 4.11D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.49356544659 IErMin= 7 ErrMin= 4.11D-06

ErrMax= 4.11D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.74D-08 BMatP= 5.91D-07

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

Coeff-Com: 0.282D-03-0.505D-02 0.544D-03 0.317D-01 0.135D+00 0.196D+00

Coeff-Com: 0.642D+00

Coeff: 0.282D-03-0.505D-02 0.544D-03 0.317D-01 0.135D+00 0.196D+00

Coeff: 0.642D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=1.26D-07 MaxDP=7.89D-06 DE=-1.52D-07 OVMax= 2.98D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.12D-07 CP: 1.00D+00 1.10D+00 9.34D-01 7.19D-01 7.58D-01

CP: 6.13D-01 9.33D-01

E= -1914.49356545176 Delta-E= -0.000000005169 Rises=F Damp=F

DIIS: error= 2.21D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.49356545176 IErMin= 8 ErrMin= 2.21D-06

ErrMax= 2.21D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.28D-09 BMatP= 1.74D-08

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

Coeff-Com: -0.639D-04 0.155D-02-0.298D-02-0.137D-01-0.470D-01-0.276D-01

Coeff-Com: 0.401D+00 0.689D+00

Coeff: -0.639D-04 0.155D-02-0.298D-02-0.137D-01-0.470D-01-0.276D-01

Coeff: 0.401D+00 0.689D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=7.47D-08 MaxDP=4.76D-06 DE=-5.17D-09 OVMax= 1.82D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 4.54D-08 CP: 1.00D+00 1.10D+00 9.34D-01 7.18D-01 7.63D-01

CP: 6.32D-01 1.14D+00 7.93D-01

E= -1914.49356545501 Delta-E= -0.000000003255 Rises=F Damp=F

DIIS: error= 1.23D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.49356545501 IErMin= 9 ErrMin= 1.23D-06

ErrMax= 1.23D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.85D-10 BMatP= 7.28D-09

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

Coeff-Com: -0.578D-04 0.118D-02-0.111D-02-0.877D-02-0.338D-01-0.348D-01

Coeff-Com: 0.673D-01 0.254D+00 0.756D+00

Coeff: -0.578D-04 0.118D-02-0.111D-02-0.877D-02-0.338D-01-0.348D-01

Coeff: 0.673D-01 0.254D+00 0.756D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=3.66D-08 MaxDP=2.10D-06 DE=-3.26D-09 OVMax= 1.04D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 2.59D-08 CP: 1.00D+00 1.10D+00 9.34D-01 7.18D-01 7.62D-01

CP: 6.46D-01 1.17D+00 9.76D-01 1.19D+00

E= -1914.49356545591 Delta-E= -0.000000000895 Rises=F Damp=F

DIIS: error= 1.06D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.49356545591 IErMin=10 ErrMin= 1.06D-06

ErrMax= 1.06D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.91D-10 BMatP= 9.85D-10

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

Coeff-Com: 0.485D-05-0.288D-03 0.143D-02 0.374D-02 0.960D-02-0.484D-02

Coeff-Com: -0.242D+00-0.317D+00 0.572D+00 0.978D+00

Coeff: 0.485D-05-0.288D-03 0.143D-02 0.374D-02 0.960D-02-0.484D-02

Coeff: -0.242D+00-0.317D+00 0.572D+00 0.978D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=4.02D-08 MaxDP=1.88D-06 DE=-8.95D-10 OVMax= 1.33D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.29D-08 CP: 1.00D+00 1.10D+00 9.34D-01 7.18D-01 7.63D-01

CP: 6.53D-01 1.25D+00 1.08D+00 1.87D+00 1.15D+00

E= -1914.49356545648 Delta-E= -0.000000000571 Rises=F Damp=F

DIIS: error= 3.66D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.49356545648 IErMin=11 ErrMin= 3.66D-07

ErrMax= 3.66D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.41D-11 BMatP= 5.91D-10

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

Coeff-Com: 0.103D-04-0.299D-03 0.820D-03 0.295D-02 0.917D-02 0.287D-02

Coeff-Com: -0.120D+00-0.184D+00 0.152D+00 0.453D+00 0.684D+00

Coeff: 0.103D-04-0.299D-03 0.820D-03 0.295D-02 0.917D-02 0.287D-02

Coeff: -0.120D+00-0.184D+00 0.152D+00 0.453D+00 0.684D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=1.09D-08 MaxDP=5.52D-07 DE=-5.71D-10 OVMax= 4.06D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 5.80D-09 CP: 1.00D+00 1.10D+00 9.34D-01 7.19D-01 7.63D-01

CP: 6.53D-01 1.26D+00 1.12D+00 2.01D+00 1.34D+00

CP: 1.08D+00

E= -1914.49356545651 Delta-E= -0.000000000032 Rises=F Damp=F

DIIS: error= 1.62D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.49356545651 IErMin=12 ErrMin= 1.62D-07

ErrMax= 1.62D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.71D-11 BMatP= 8.41D-11

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

Coeff-Com: 0.404D-05-0.702D-04-0.118D-04 0.405D-03 0.194D-02 0.317D-02

Coeff-Com: 0.113D-01-0.819D-03-0.968D-01-0.608D-01 0.373D+00 0.768D+00

Coeff: 0.404D-05-0.702D-04-0.118D-04 0.405D-03 0.194D-02 0.317D-02

Coeff: 0.113D-01-0.819D-03-0.968D-01-0.608D-01 0.373D+00 0.768D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=6.19D-09 MaxDP=3.04D-07 DE=-3.18D-11 OVMax= 2.20D-06

Error on total polarization charges = 0.08622

SCF Done: E(UB3LYP) = -1914.49356546 A.U. after 12 cycles

NFock= 12 Conv=0.62D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7585 S= 0.5043

<L.S>= 0.000000000000E+00

KE= 1.906574206226D+03 PE=-1.517702068248D+04 EE= 6.009926220834D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.24

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7585, after 0.7500

Leave Link 502 at Sun Aug 18 14:36:49 2019, MaxMem= 2013265920 cpu: 3430.5

(Enter /home/kira/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 = 183

Leave Link 701 at Sun Aug 18 14:37:07 2019, MaxMem= 2013265920 cpu: 140.0

(Enter /home/kira/g09/l702.exe)

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

Leave Link 702 at Sun Aug 18 14:37:07 2019, MaxMem= 2013265920 cpu: 0.2

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 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= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

Petite list used in FoFCou.

Leave Link 703 at Sun Aug 18 14:38:23 2019, MaxMem= 2013265920 cpu: 612.1

(Enter /home/kira/g09/l716.exe)

Dipole =-1.12233971D-03-1.38174515D-01 3.08197911D-13

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000077018 0.000066677 -0.000032488

2 6 -0.000131867 0.000049199 0.000518661

3 7 -0.000294389 -0.000476994 -0.000000000

4 6 -0.000131867 0.000049199 -0.000518661

5 6 0.000077018 0.000066677 0.000032488

6 6 0.000074097 0.000234017 0.000144080

7 6 0.000547449 0.000208313 0.000083328

8 7 -0.000015342 -0.000494298 0.000140919

9 6 -0.000511733 0.000242786 0.000123639

10 6 0.000118605 -0.000069652 -0.000039264

11 6 -0.000053747 -0.000033762 -0.000037570

12 6 0.000074097 0.000234017 -0.000144080

13 6 0.000547449 0.000208313 -0.000083328

14 6 -0.000053747 -0.000033762 0.000037570

15 6 0.000118605 -0.000069652 0.000039264

16 6 -0.000511733 0.000242786 -0.000123639

17 7 -0.000015342 -0.000494298 -0.000140919

18 6 -0.000100903 0.000224118 -0.000092737

19 6 0.000097480 0.000048831 0.000515610

20 6 -0.000088077 0.000040875 -0.000086946

21 6 -0.000088077 0.000040875 0.000086946

22 6 0.000097480 0.000048831 -0.000515610

23 7 0.000264777 -0.000397596 0.000000000

24 6 -0.000100903 0.000224118 0.000092737

25 6 -0.000164934 -0.000284671 0.000186079

26 6 0.000244386 0.000000248 -0.000143292

27 6 -0.000014769 0.000061119 0.000137464

28 6 -0.000004311 -0.000023991 -0.000011500

29 6 -0.000133896 0.000025764 0.000037033

30 6 0.000239311 0.000133562 -0.000187709

31 6 -0.000004311 -0.000023991 0.000011500

32 6 -0.000014769 0.000061119 -0.000137464

33 6 0.000244386 0.000000248 0.000143292

34 6 -0.000164934 -0.000284671 -0.000186079

35 6 0.000239311 0.000133562 0.000187709

36 6 -0.000133896 0.000025764 -0.000037033

37 6 0.000173121 -0.000274962 0.000209287

38 6 -0.000245634 0.000107559 -0.000221658

39 6 0.000148956 0.000031717 0.000025628

40 6 -0.000000336 -0.000020242 -0.000004127

41 6 0.000003843 0.000055031 0.000145408

42 6 -0.000284609 0.000008124 -0.000143093

43 6 0.000173121 -0.000274962 -0.000209287

44 6 -0.000245634 0.000107559 0.000221658

45 6 0.000148956 0.000031717 -0.000025628

46 6 -0.000000336 -0.000020242 0.000004127

47 6 0.000003843 0.000055031 -0.000145408

48 6 -0.000284609 0.000008124 0.000143093

49 1 -0.000013911 -0.000091706 -0.000046756

50 1 -0.000013911 -0.000091706 0.000046756

51 1 0.000084137 0.000016996 -0.000021174

52 1 -0.000055704 0.000024616 -0.000039025

53 1 -0.000055704 0.000024616 0.000039025

54 1 0.000084137 0.000016996 0.000021174

55 1 0.000032572 -0.000090172 -0.000059036

56 1 0.000032572 -0.000090172 0.000059036

57 1 -0.000018406 0.000020559 -0.000039326

58 1 0.000029870 -0.000004593 0.000003382

59 1 0.000003136 -0.000001202 -0.000009525

60 1 -0.000008550 0.000003915 -0.000031572

61 1 0.000010434 -0.000019136 0.000029445

62 1 0.000003136 -0.000001202 0.000009525

63 1 0.000029870 -0.000004593 -0.000003382

64 1 -0.000018406 0.000020559 0.000039326

65 1 0.000010434 -0.000019136 -0.000029445

66 1 -0.000008550 0.000003915 0.000031572

67 1 -0.000025616 -0.000007934 0.000027217

68 1 0.000004060 0.000006440 -0.000032541

69 1 -0.000004043 0.000000446 -0.000011095

70 1 -0.000029438 -0.000005604 -0.000002121

71 1 0.000024866 0.000020176 -0.000063865

72 1 -0.000025616 -0.000007934 -0.000027217

73 1 0.000004060 0.000006440 0.000032541

74 1 -0.000004043 0.000000446 0.000011095

75 1 -0.000029438 -0.000005604 0.000002121

76 1 0.000024866 0.000020176 0.000063865

77 1 0.000039692 0.000237988 0.000000000

78 1 -0.000025106 0.000218277 -0.000000000

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

Cartesian Forces: Max 0.000547449 RMS 0.000157283

Leave Link 716 at Sun Aug 18 14:38:23 2019, MaxMem= 2013265920 cpu: 0.2

(Enter /home/kira/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 0.000406425 RMS 0.000107222

Search for a local minimum.

Step number 6 out of a maximum of 452

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

RMS Force = .10722D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 3 4 5 6

DE= -4.29D-05 DEPred=-1.24D-04 R= 3.46D-01

Trust test= 3.46D-01 RLast= 2.26D-01 DXMaxT set to 9.59D-01

ITU= 0 1 1 1 1 0

Eigenvalues --- 0.00640 0.00983 0.00988 0.00990 0.01423

Eigenvalues --- 0.01606 0.01617 0.01621 0.01634 0.01660

Eigenvalues --- 0.01723 0.01723 0.01724 0.01728 0.01733

Eigenvalues --- 0.01748 0.01751 0.01772 0.01791 0.01824

Eigenvalues --- 0.01837 0.01846 0.01856 0.01879 0.01891

Eigenvalues --- 0.01902 0.01928 0.01943 0.01955 0.01987

Eigenvalues --- 0.01996 0.02011 0.02020 0.02027 0.02068

Eigenvalues --- 0.02068 0.02070 0.02070 0.02074 0.02086

Eigenvalues --- 0.02102 0.02112 0.02118 0.02118 0.02119

Eigenvalues --- 0.02122 0.02130 0.02130 0.02132 0.02132

Eigenvalues --- 0.02132 0.02136 0.02160 0.02160 0.02160

Eigenvalues --- 0.02161 0.02162 0.02162 0.02162 0.02173

Eigenvalues --- 0.02173 0.02173 0.02174 0.02181 0.02181

Eigenvalues --- 0.02181 0.02183 0.02186 0.02187 0.02187

Eigenvalues --- 0.02188 0.02217 0.02217 0.02224 0.03230

Eigenvalues --- 0.15882 0.15903 0.15910 0.15997 0.15997

Eigenvalues --- 0.15998 0.15998 0.15998 0.15999 0.15999

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16002 0.16009 0.16086

Eigenvalues --- 0.21547 0.22000 0.22000 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22001 0.22056 0.22759

Eigenvalues --- 0.22774 0.22818 0.22834 0.23473 0.23473

Eigenvalues --- 0.23476 0.23540 0.23758 0.24436 0.24736

Eigenvalues --- 0.24862 0.24947 0.24976 0.24988 0.24994

Eigenvalues --- 0.24995 0.24999 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25001 0.25056

Eigenvalues --- 0.25970 0.27652 0.34159 0.34182 0.34206

Eigenvalues --- 0.34613 0.35410 0.35413 0.35413 0.35413

Eigenvalues --- 0.35414 0.35415 0.35416 0.35416 0.35416

Eigenvalues --- 0.35416 0.35416 0.35422 0.35506 0.35507

Eigenvalues --- 0.35508 0.35525 0.35542 0.35545 0.35547

Eigenvalues --- 0.35713 0.36056 0.36057 0.36058 0.36101

Eigenvalues --- 0.36250 0.36251 0.36251 0.36266 0.37117

Eigenvalues --- 0.37157 0.37257 0.37292 0.37558 0.39133

Eigenvalues --- 0.39746 0.39910 0.40265 0.40425 0.40466

Eigenvalues --- 0.40623 0.41779 0.41784 0.41795 0.42055

Eigenvalues --- 0.42094 0.42095 0.42097 0.42103 0.42733

Eigenvalues --- 0.43273 0.44661 0.45403 0.45568 0.45573

Eigenvalues --- 0.45585 0.45592 0.45709 0.45770 0.45845

Eigenvalues --- 0.45862 0.45931 0.45939 0.45942 0.45949

Eigenvalues --- 0.45971 0.46660 0.46660 0.46661 0.46669

Eigenvalues --- 0.47073 0.47079 0.47086 0.47468 0.47640

Eigenvalues --- 0.48192 0.48278 0.49335 0.49434 0.49976

Eigenvalues --- 0.50707 0.50811 0.54925

En-DIIS/RFO-DIIS IScMMF= 0 using points: 6 5 4 3 2

RFO step: Lambda=-1.77114246D-05.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 4.14D-04 SmlDif= 1.00D-05

RMS Error= 0.5117220285D-03 NUsed= 5 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.58857 0.33255 -0.03439 -0.03229 0.14556

Iteration 1 RMS(Cart)= 0.04490750 RMS(Int)= 0.00049933

Iteration 2 RMS(Cart)= 0.00088169 RMS(Int)= 0.00007018

Iteration 3 RMS(Cart)= 0.00000035 RMS(Int)= 0.00007018

ITry= 1 IFail=0 DXMaxC= 1.60D-01 DCOld= 1.00D+10 DXMaxT= 9.59D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.21D-08 for atom 50.

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

(Linear) (Quad) (Total)

R1 2.72704 0.00007 -0.00013 0.00006 -0.00011 2.72693

R2 2.57374 -0.00004 0.00032 -0.00024 -0.00002 2.57371

R3 2.03849 -0.00003 -0.00008 -0.00007 -0.00015 2.03834

R4 2.61801 0.00027 0.00034 -0.00001 0.00041 2.61842

R5 2.61854 -0.00029 0.00060 -0.00039 0.00021 2.61875

R6 2.61801 0.00027 0.00034 -0.00001 0.00041 2.61842

R7 1.91006 -0.00004 -0.00020 0.00011 -0.00009 1.90996

R8 2.72704 0.00007 -0.00013 0.00006 -0.00011 2.72693

R9 2.61854 -0.00029 0.00060 -0.00039 0.00021 2.61875

R10 2.03849 -0.00003 -0.00008 -0.00007 -0.00015 2.03834

R11 2.70298 0.00002 0.00103 -0.00033 0.00070 2.70368

R12 2.82114 0.00015 -0.00128 0.00034 -0.00093 2.82021

R13 2.59249 0.00041 0.00043 0.00024 0.00075 2.59324

R14 2.71575 0.00009 -0.00013 0.00010 -0.00006 2.71569

R15 2.59258 0.00038 0.00042 0.00020 0.00070 2.59328

R16 2.71560 0.00016 -0.00006 0.00017 0.00008 2.71568

R17 2.70266 0.00014 0.00122 -0.00023 0.00099 2.70365

R18 2.60038 0.00007 0.00023 -0.00023 -0.00010 2.60028

R19 2.04093 -0.00003 0.00007 -0.00011 -0.00004 2.04089

R20 2.04086 -0.00000 0.00010 -0.00007 0.00003 2.04089

R21 2.70298 0.00002 0.00103 -0.00033 0.00070 2.70368

R22 2.82114 0.00015 -0.00128 0.00034 -0.00093 2.82021

R23 2.71575 0.00009 -0.00013 0.00010 -0.00006 2.71569

R24 2.59249 0.00041 0.00043 0.00024 0.00075 2.59324

R25 2.60038 0.00007 0.00023 -0.00023 -0.00010 2.60028

R26 2.04086 -0.00000 0.00010 -0.00007 0.00003 2.04089

R27 2.71560 0.00016 -0.00006 0.00017 0.00008 2.71568

R28 2.04093 -0.00003 0.00007 -0.00011 -0.00004 2.04089

R29 2.59258 0.00038 0.00042 0.00020 0.00070 2.59328

R30 2.70266 0.00014 0.00122 -0.00023 0.00099 2.70365

R31 2.61822 -0.00015 0.00086 -0.00032 0.00054 2.61876

R32 2.82110 0.00022 -0.00139 0.00049 -0.00091 2.82019

R33 2.72702 0.00008 -0.00015 0.00008 -0.00010 2.72692

R34 2.61780 0.00033 0.00035 0.00007 0.00051 2.61832

R35 2.57383 -0.00006 0.00028 -0.00025 -0.00008 2.57375

R36 2.03855 -0.00005 -0.00011 -0.00009 -0.00020 2.03835

R37 2.72702 0.00008 -0.00015 0.00008 -0.00010 2.72692

R38 2.03855 -0.00005 -0.00011 -0.00009 -0.00020 2.03835

R39 2.61780 0.00033 0.00035 0.00007 0.00051 2.61832

R40 2.61822 -0.00015 0.00086 -0.00032 0.00054 2.61876

R41 1.91001 -0.00002 -0.00026 0.00016 -0.00010 1.90991

R42 2.82110 0.00022 -0.00139 0.00049 -0.00091 2.82019

R43 2.64581 0.00021 0.00104 0.00001 0.00105 2.64686

R44 2.64835 0.00001 0.00079 -0.00020 0.00059 2.64894

R45 2.63459 -0.00009 -0.00026 -0.00015 -0.00041 2.63418

R46 2.04993 -0.00001 -0.00012 0.00002 -0.00010 2.04983

R47 2.63362 0.00001 0.00005 0.00002 0.00007 2.63369

R48 2.05082 0.00002 0.00005 -0.00000 0.00005 2.05087

R49 2.63640 -0.00001 0.00002 -0.00001 0.00002 2.63642

R50 2.05048 0.00001 0.00001 -0.00000 0.00000 2.05049

R51 2.63171 -0.00009 -0.00033 -0.00015 -0.00048 2.63123

R52 2.05083 0.00002 0.00006 -0.00001 0.00005 2.05087

R53 2.04958 0.00001 -0.00011 0.00005 -0.00007 2.04951

R54 2.63362 0.00001 0.00005 0.00002 0.00007 2.63369

R55 2.63640 -0.00001 0.00002 -0.00001 0.00002 2.63642

R56 2.05048 0.00001 0.00001 -0.00000 0.00000 2.05049

R57 2.63459 -0.00009 -0.00026 -0.00015 -0.00041 2.63418

R58 2.05082 0.00002 0.00005 -0.00000 0.00005 2.05087

R59 2.64581 0.00021 0.00104 0.00001 0.00105 2.64686

R60 2.04993 -0.00001 -0.00012 0.00002 -0.00010 2.04983

R61 2.64835 0.00001 0.00079 -0.00020 0.00059 2.64894

R62 2.63171 -0.00009 -0.00033 -0.00015 -0.00048 2.63123

R63 2.04958 0.00001 -0.00011 0.00005 -0.00007 2.04951

R64 2.05083 0.00002 0.00006 -0.00001 0.00005 2.05087

R65 2.64820 0.00005 0.00093 -0.00019 0.00074 2.64894

R66 2.64567 0.00025 0.00115 0.00003 0.00118 2.64685

R67 2.63173 -0.00008 -0.00037 -0.00013 -0.00050 2.63123

R68 2.04964 -0.00001 -0.00015 0.00003 -0.00012 2.04951

R69 2.63640 -0.00001 0.00003 -0.00001 0.00002 2.63642

R70 2.05083 0.00001 0.00006 -0.00001 0.00004 2.05087

R71 2.63365 -0.00001 0.00004 0.00000 0.00004 2.63369

R72 2.05048 0.00001 0.00001 -0.00000 0.00001 2.05049

R73 2.63461 -0.00009 -0.00029 -0.00014 -0.00043 2.63418

R74 2.05082 0.00001 0.00005 -0.00001 0.00004 2.05087

R75 2.04997 -0.00002 -0.00015 0.00001 -0.00014 2.04983

R76 2.64820 0.00005 0.00093 -0.00019 0.00074 2.64894

R77 2.64567 0.00025 0.00115 0.00003 0.00118 2.64685

R78 2.63173 -0.00008 -0.00037 -0.00013 -0.00050 2.63123

R79 2.04964 -0.00001 -0.00015 0.00003 -0.00012 2.04951

R80 2.63640 -0.00001 0.00003 -0.00001 0.00002 2.63642

R81 2.05083 0.00001 0.00006 -0.00001 0.00004 2.05087

R82 2.63365 -0.00001 0.00004 0.00000 0.00004 2.63369

R83 2.05048 0.00001 0.00001 -0.00000 0.00001 2.05049

R84 2.63461 -0.00009 -0.00029 -0.00014 -0.00043 2.63418

R85 2.05082 0.00001 0.00005 -0.00001 0.00004 2.05087

R86 2.04997 -0.00002 -0.00015 0.00001 -0.00014 2.04983

A1 1.89585 0.00007 0.00029 -0.00014 0.00018 1.89603

A2 2.17289 -0.00000 0.00034 0.00020 0.00052 2.17340

A3 2.21439 -0.00007 -0.00065 -0.00005 -0.00071 2.21368

A4 1.84773 -0.00005 -0.00074 0.00046 -0.00024 1.84750

A5 2.21796 -0.00009 0.00120 -0.00045 0.00048 2.21844

A6 2.21736 0.00014 -0.00042 0.00000 -0.00017 2.21719

A7 1.93760 -0.00005 0.00077 -0.00063 0.00009 1.93769

A8 2.17084 0.00004 -0.00027 0.00063 0.00039 2.17123

A9 2.17084 0.00004 -0.00027 0.00063 0.00039 2.17123

A10 1.84773 -0.00005 -0.00074 0.00046 -0.00024 1.84750

A11 2.21736 0.00014 -0.00042 0.00000 -0.00017 2.21719

A12 2.21796 -0.00009 0.00120 -0.00045 0.00048 2.21844

A13 1.89585 0.00007 0.00029 -0.00014 0.00018 1.89603

A14 2.21439 -0.00007 -0.00065 -0.00005 -0.00071 2.21368

A15 2.17289 -0.00000 0.00034 0.00020 0.00052 2.17340

A16 2.19390 -0.00014 -0.00217 0.00001 -0.00181 2.19209

A17 2.04274 -0.00012 0.00140 -0.00055 0.00067 2.04342

A18 2.04654 0.00025 0.00077 0.00055 0.00114 2.04768

A19 2.19207 0.00008 0.00009 -0.00045 -0.00009 2.19198

A20 2.16054 0.00012 0.00058 0.00032 0.00062 2.16116

A21 1.93056 -0.00020 -0.00067 0.00013 -0.00051 1.93004

A22 1.84784 0.00017 0.00073 -0.00021 0.00045 1.84829

A23 1.93071 -0.00026 -0.00076 0.00004 -0.00069 1.93002

A24 2.19219 0.00005 0.00004 -0.00048 -0.00016 2.19204

A25 2.16025 0.00021 0.00072 0.00044 0.00088 2.16113

A26 1.85765 0.00017 0.00036 0.00009 0.00048 1.85813

A27 2.20340 -0.00000 -0.00014 0.00033 0.00018 2.20358

A28 2.22206 -0.00017 -0.00024 -0.00042 -0.00067 2.22139

A29 1.85782 0.00012 0.00027 -0.00002 0.00027 1.85809

A30 2.20339 0.00001 -0.00012 0.00037 0.00023 2.20362

A31 2.22190 -0.00013 -0.00016 -0.00034 -0.00052 2.22138

A32 2.19390 -0.00014 -0.00217 0.00001 -0.00181 2.19209

A33 2.04274 -0.00012 0.00140 -0.00055 0.00067 2.04342

A34 2.04654 0.00025 0.00077 0.00055 0.00114 2.04768

A35 2.16054 0.00012 0.00058 0.00032 0.00062 2.16116

A36 2.19207 0.00008 0.00009 -0.00045 -0.00009 2.19198

A37 1.93056 -0.00020 -0.00067 0.00013 -0.00051 1.93004

A38 1.85782 0.00012 0.00027 -0.00002 0.00027 1.85809

A39 2.20339 0.00001 -0.00012 0.00037 0.00023 2.20362

A40 2.22190 -0.00013 -0.00016 -0.00034 -0.00052 2.22138

A41 1.85765 0.00017 0.00036 0.00009 0.00048 1.85813

A42 2.22206 -0.00017 -0.00024 -0.00042 -0.00067 2.22139

A43 2.20340 -0.00000 -0.00014 0.00033 0.00018 2.20358

A44 1.93071 -0.00026 -0.00076 0.00004 -0.00069 1.93002

A45 2.16025 0.00021 0.00072 0.00044 0.00088 2.16113

A46 2.19219 0.00005 0.00004 -0.00048 -0.00016 2.19204

A47 1.84784 0.00017 0.00073 -0.00021 0.00045 1.84829

A48 2.19409 -0.00018 -0.00233 -0.00003 -0.00198 2.19211

A49 2.04632 0.00030 0.00101 0.00058 0.00140 2.04772

A50 2.04277 -0.00011 0.00132 -0.00054 0.00058 2.04335

A51 2.21795 -0.00005 0.00122 -0.00040 0.00052 2.21846

A52 2.21721 0.00016 -0.00029 0.00001 -0.00001 2.21720

A53 1.84790 -0.00010 -0.00088 0.00041 -0.00044 1.84746

A54 1.89574 0.00010 0.00034 -0.00011 0.00028 1.89601

A55 2.17291 -0.00002 0.00032 0.00015 0.00046 2.17337

A56 2.21448 -0.00008 -0.00070 -0.00003 -0.00075 2.21373

A57 1.89574 0.00010 0.00034 -0.00011 0.00028 1.89601

A58 2.21448 -0.00008 -0.00070 -0.00003 -0.00075 2.21373

A59 2.17291 -0.00002 0.00032 0.00015 0.00046 2.17337

A60 1.84790 -0.00010 -0.00088 0.00041 -0.00044 1.84746

A61 2.21795 -0.00005 0.00122 -0.00040 0.00052 2.21846

A62 2.21721 0.00016 -0.00029 0.00001 -0.00001 2.21720

A63 1.93749 -0.00001 0.00094 -0.00060 0.00029 1.93778

A64 2.17103 0.00001 -0.00024 0.00056 0.00036 2.17139

A65 2.17103 0.00001 -0.00024 0.00056 0.00036 2.17139

A66 2.19409 -0.00018 -0.00233 -0.00003 -0.00198 2.19211

A67 2.04632 0.00030 0.00101 0.00058 0.00140 2.04772

A68 2.04277 -0.00011 0.00132 -0.00054 0.00058 2.04335

A69 2.11296 -0.00006 0.00112 -0.00053 0.00059 2.11355

A70 2.10264 0.00025 0.00052 0.00033 0.00085 2.10349

A71 2.06758 -0.00018 -0.00164 0.00020 -0.00144 2.06615

A72 2.10859 0.00011 0.00081 -0.00004 0.00077 2.10936

A73 2.08207 -0.00004 -0.00032 0.00008 -0.00024 2.08184

A74 2.09251 -0.00007 -0.00051 -0.00004 -0.00054 2.09197

A75 2.09747 -0.00003 0.00020 -0.00017 0.00003 2.09750

A76 2.08914 0.00003 -0.00011 0.00009 -0.00002 2.08911

A77 2.09657 0.00000 -0.00009 0.00008 -0.00001 2.09656

A78 2.08658 -0.00001 -0.00047 0.00017 -0.00030 2.08628

A79 2.09848 0.00001 0.00022 -0.00007 0.00015 2.09863

A80 2.09813 0.00000 0.00025 -0.00010 0.00015 2.09828

A81 2.09736 0.00003 0.00024 -0.00005 0.00020 2.09756

A82 2.09612 -0.00002 -0.00011 0.00004 -0.00007 2.09605

A83 2.08970 -0.00000 -0.00014 0.00001 -0.00013 2.08957

A84 2.10877 0.00010 0.00086 -0.00011 0.00075 2.10952

A85 2.08188 -0.00006 -0.00039 0.00005 -0.00034 2.08155

A86 2.09251 -0.00004 -0.00048 0.00007 -0.00041 2.09209

A87 2.08658 -0.00001 -0.00047 0.00017 -0.00030 2.08628

A88 2.09848 0.00001 0.00022 -0.00007 0.00015 2.09863

A89 2.09813 0.00000 0.00025 -0.00010 0.00015 2.09828

A90 2.09747 -0.00003 0.00020 -0.00017 0.00003 2.09750

A91 2.09657 0.00000 -0.00009 0.00008 -0.00001 2.09656

A92 2.08914 0.00003 -0.00011 0.00009 -0.00002 2.08911

A93 2.10859 0.00011 0.00081 -0.00004 0.00077 2.10936

A94 2.09251 -0.00007 -0.00051 -0.00004 -0.00054 2.09197

A95 2.08207 -0.00004 -0.00032 0.00008 -0.00024 2.08184

A96 2.11296 -0.00006 0.00112 -0.00053 0.00059 2.11355

A97 2.10264 0.00025 0.00052 0.00033 0.00085 2.10349

A98 2.06758 -0.00018 -0.00164 0.00020 -0.00144 2.06615

A99 2.10877 0.00010 0.00086 -0.00011 0.00075 2.10952

A100 2.08188 -0.00006 -0.00039 0.00005 -0.00034 2.08155

A101 2.09251 -0.00004 -0.00048 0.00007 -0.00041 2.09209

A102 2.09736 0.00003 0.00024 -0.00005 0.00020 2.09756

A103 2.09612 -0.00002 -0.00011 0.00004 -0.00007 2.09605

A104 2.08970 -0.00000 -0.00014 0.00001 -0.00013 2.08957

A105 2.10247 0.00027 0.00062 0.00036 0.00098 2.10346

A106 2.11292 -0.00005 0.00120 -0.00055 0.00065 2.11357

A107 2.06779 -0.00022 -0.00182 0.00019 -0.00163 2.06616

A108 2.10869 0.00010 0.00094 -0.00012 0.00082 2.10951

A109 2.08188 -0.00006 -0.00039 0.00005 -0.00034 2.08155

A110 2.09259 -0.00005 -0.00056 0.00008 -0.00049 2.09210

A111 2.09732 0.00003 0.00028 -0.00004 0.00023 2.09756

A112 2.08970 -0.00000 -0.00016 0.00003 -0.00013 2.08957

A113 2.09616 -0.00003 -0.00012 0.00001 -0.00011 2.09605

A114 2.08662 -0.00001 -0.00052 0.00018 -0.00034 2.08628

A115 2.09810 0.00000 0.00027 -0.00010 0.00017 2.09827

A116 2.09846 0.00001 0.00025 -0.00009 0.00016 2.09863

A117 2.09745 -0.00003 0.00023 -0.00018 0.00004 2.09749

A118 2.09659 -0.00000 -0.00010 0.00007 -0.00003 2.09656

A119 2.08914 0.00003 -0.00013 0.00011 -0.00002 2.08912

A120 2.10848 0.00012 0.00090 -0.00003 0.00087 2.10935

A121 2.08207 -0.00004 -0.00032 0.00008 -0.00023 2.08183

A122 2.09263 -0.00008 -0.00059 -0.00005 -0.00065 2.09198

A123 2.10247 0.00027 0.00062 0.00036 0.00098 2.10346

A124 2.11292 -0.00005 0.00120 -0.00055 0.00065 2.11357

A125 2.06779 -0.00022 -0.00182 0.00019 -0.00163 2.06616

A126 2.10869 0.00010 0.00094 -0.00012 0.00082 2.10951

A127 2.08188 -0.00006 -0.00039 0.00005 -0.00034 2.08155

A128 2.09259 -0.00005 -0.00056 0.00008 -0.00049 2.09210

A129 2.09732 0.00003 0.00028 -0.00004 0.00023 2.09756

A130 2.08970 -0.00000 -0.00016 0.00003 -0.00013 2.08957

A131 2.09616 -0.00003 -0.00012 0.00001 -0.00011 2.09605

A132 2.08662 -0.00001 -0.00052 0.00018 -0.00034 2.08628

A133 2.09810 0.00000 0.00027 -0.00010 0.00017 2.09827

A134 2.09846 0.00001 0.00025 -0.00009 0.00016 2.09863

A135 2.09745 -0.00003 0.00023 -0.00018 0.00004 2.09749

A136 2.09659 -0.00000 -0.00010 0.00007 -0.00003 2.09656

A137 2.08914 0.00003 -0.00013 0.00011 -0.00002 2.08912

A138 2.10848 0.00012 0.00090 -0.00003 0.00087 2.10935

A139 2.08207 -0.00004 -0.00032 0.00008 -0.00023 2.08183

A140 2.09263 -0.00008 -0.00059 -0.00005 -0.00065 2.09198

D1 -0.00127 0.00010 0.00469 0.00105 0.00576 0.00448

D2 3.12368 0.00017 0.00985 0.00195 0.01181 3.13549

D3 -3.13192 0.00006 0.00650 0.00053 0.00703 -3.12489

D4 -0.00696 0.00013 0.01165 0.00142 0.01308 0.00611

D5 0.00000 -0.00000 -0.00000 0.00000 0.00000 0.00000

D6 -3.13031 -0.00004 0.00185 -0.00054 0.00130 -3.12901

D7 3.13031 0.00004 -0.00185 0.00054 -0.00130 3.12901

D8 -0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.00213 -0.00017 -0.00787 -0.00177 -0.00963 -0.00750

D10 3.05241 0.00013 -0.00446 0.00569 0.00123 3.05364

D11 -3.12283 -0.00024 -0.01302 -0.00266 -0.01569 -3.13852

D12 -0.07255 0.00006 -0.00961 0.00480 -0.00482 -0.07737

D13 -3.08601 0.00007 0.00545 0.00094 0.00639 -3.07962

D14 0.05352 0.00009 0.00539 0.00097 0.00637 0.05988

D15 0.03553 0.00016 0.01166 0.00203 0.01369 0.04922

D16 -3.10813 0.00017 0.01160 0.00206 0.01366 -3.09447

D17 -0.00213 0.00017 0.00787 0.00177 0.00963 0.00750

D18 3.12283 0.00024 0.01302 0.00266 0.01569 3.13852

D19 -3.05241 -0.00013 0.00446 -0.00569 -0.00123 -3.05364

D20 0.07255 -0.00006 0.00961 -0.00480 0.00482 0.07737

D21 0.00127 -0.00010 -0.00469 -0.00105 -0.00576 -0.00448

D22 3.13192 -0.00006 -0.00650 -0.00053 -0.00703 3.12489

D23 -3.12368 -0.00017 -0.00985 -0.00195 -0.01181 -3.13549

D24 0.00696 -0.00013 -0.01165 -0.00142 -0.01308 -0.00611

D25 -0.03553 -0.00016 -0.01166 -0.00203 -0.01369 -0.04922

D26 3.10813 -0.00017 -0.01160 -0.00206 -0.01366 3.09447

D27 3.08601 -0.00007 -0.00545 -0.00094 -0.00639 3.07962

D28 -0.05352 -0.00009 -0.00539 -0.00097 -0.00637 -0.05988

D29 -0.09598 -0.00016 -0.02425 0.00152 -0.02273 -0.11872

D30 3.03720 -0.00006 -0.01715 0.00155 -0.01560 3.02160

D31 3.04354 -0.00015 -0.02430 0.00155 -0.02276 3.02078

D32 -0.10647 -0.00005 -0.01721 0.00158 -0.01562 -0.12209

D33 -1.13959 0.00009 0.02564 -0.00301 0.02263 -1.11696

D34 2.00249 0.00010 0.02631 -0.00264 0.02366 2.02615

D35 2.00389 0.00008 0.02569 -0.00304 0.02266 2.02655

D36 -1.13721 0.00009 0.02636 -0.00267 0.02369 -1.11352

D37 -3.13018 0.00001 0.00783 -0.00104 0.00680 -3.12337

D38 0.01888 -0.00008 0.00154 -0.00107 0.00047 0.01935

D39 3.13712 -0.00004 -0.00718 0.00058 -0.00661 3.13051

D40 -0.01721 -0.00005 -0.00818 0.00062 -0.00757 -0.02478

D41 -0.01178 0.00005 -0.00101 0.00061 -0.00041 -0.01219

D42 3.11708 0.00004 -0.00202 0.00065 -0.00137 3.11571

D43 -0.01897 0.00009 -0.00148 0.00114 -0.00035 -0.01932

D44 3.13067 -0.00002 -0.00832 0.00089 -0.00745 3.12322

D45 0.01201 -0.00006 0.00087 -0.00078 0.00010 0.01210

D46 -3.11699 -0.00004 0.00205 -0.00079 0.00126 -3.11574

D47 -3.13746 0.00004 0.00757 -0.00054 0.00705 -3.13041

D48 0.01673 0.00006 0.00875 -0.00055 0.00821 0.02493

D49 0.09544 0.00017 0.02497 -0.00167 0.02332 0.11876

D50 -3.04429 0.00016 0.02581 -0.00219 0.02363 -3.02066

D51 -3.03709 0.00005 0.01726 -0.00195 0.01532 -3.02177

D52 0.10636 0.00004 0.01809 -0.00247 0.01563 0.12199

D53 -0.00013 0.00001 0.00008 0.00010 0.00018 0.00005

D54 -3.12881 0.00002 0.00110 0.00005 0.00115 -3.12766

D55 3.12869 -0.00001 -0.00112 0.00012 -0.00099 3.12771

D56 0.00001 0.00000 -0.00010 0.00008 -0.00002 -0.00001

D57 -3.03720 0.00006 0.01715 -0.00155 0.01560 -3.02160

D58 0.09598 0.00016 0.02425 -0.00152 0.02273 0.11872

D59 0.10647 0.00005 0.01721 -0.00158 0.01562 0.12209

D60 -3.04354 0.00015 0.02430 -0.00155 0.02276 -3.02078

D61 1.13959 -0.00009 -0.02564 0.00301 -0.02263 1.11696

D62 -2.00249 -0.00010 -0.02631 0.00264 -0.02366 -2.02615

D63 -2.00389 -0.00008 -0.02569 0.00304 -0.02266 -2.02655

D64 1.13721 -0.00009 -0.02636 0.00267 -0.02369 1.11352

D65 -3.13712 0.00004 0.00718 -0.00058 0.00661 -3.13051

D66 0.01721 0.00005 0.00818 -0.00062 0.00757 0.02478

D67 0.01178 -0.00005 0.00101 -0.00061 0.00041 0.01219

D68 -3.11708 -0.00004 0.00202 -0.00065 0.00137 -3.11571

D69 3.13018 -0.00001 -0.00783 0.00104 -0.00680 3.12337

D70 -0.01888 0.00008 -0.00154 0.00107 -0.00047 -0.01935

D71 0.00013 -0.00001 -0.00008 -0.00010 -0.00018 -0.00005

D72 -3.12869 0.00001 0.00112 -0.00012 0.00099 -3.12771

D73 3.12881 -0.00002 -0.00110 -0.00005 -0.00115 3.12766

D74 -0.00001 -0.00000 0.00010 -0.00008 0.00002 0.00001

D75 -0.01201 0.00006 -0.00087 0.00078 -0.00010 -0.01210

D76 3.13746 -0.00004 -0.00757 0.00054 -0.00705 3.13041

D77 3.11699 0.00004 -0.00205 0.00079 -0.00126 3.11574

D78 -0.01673 -0.00006 -0.00875 0.00055 -0.00821 -0.02493

D79 0.01897 -0.00009 0.00148 -0.00114 0.00035 0.01932

D80 -3.13067 0.00002 0.00832 -0.00089 0.00745 -3.12322

D81 3.03709 -0.00005 -0.01726 0.00195 -0.01532 3.02177

D82 -0.10636 -0.00004 -0.01809 0.00247 -0.01563 -0.12199

D83 -0.09544 -0.00017 -0.02497 0.00167 -0.02332 -0.11876

D84 3.04429 -0.00016 -0.02581 0.00219 -0.02363 3.02066

D85 3.08808 -0.00010 -0.00853 -0.00049 -0.00902 3.07906

D86 -0.03402 -0.00018 -0.01316 -0.00191 -0.01507 -0.04909

D87 -0.05165 -0.00011 -0.00769 -0.00102 -0.00872 -0.06037

D88 3.10944 -0.00019 -0.01232 -0.00243 -0.01477 3.09467

D89 -1.13967 0.00010 0.02844 -0.00210 0.02634 -1.11333

D90 2.00131 0.00009 0.02821 -0.00267 0.02554 2.02685

D91 2.00022 0.00011 0.02768 -0.00162 0.02605 2.02628

D92 -1.14198 0.00010 0.02744 -0.00219 0.02525 -1.11673

D93 -3.12451 -0.00016 -0.00849 -0.00237 -0.01088 -3.13539

D94 0.00636 -0.00013 -0.01116 -0.00150 -0.01266 -0.00630

D95 0.00091 -0.00010 -0.00464 -0.00120 -0.00586 -0.00495

D96 3.13177 -0.00006 -0.00731 -0.00032 -0.00764 3.12414

D97 3.12391 0.00023 0.01164 0.00318 0.01483 3.13874

D98 0.07047 -0.00005 0.00468 -0.00315 0.00154 0.07200

D99 -0.00152 0.00016 0.00779 0.00201 0.00980 0.00828

D100 -3.05496 -0.00012 0.00084 -0.00432 -0.00349 -3.05845

D101 -0.00000 -0.00000 -0.00000 0.00000 0.00000 0.00000

D102 3.13054 0.00004 -0.00273 0.00091 -0.00182 3.12872

D103 -3.13054 -0.00004 0.00273 -0.00091 0.00182 -3.12872

D104 0.00000 0.00000 -0.00000 0.00000 0.00000 0.00000

D105 -0.00091 0.00010 0.00464 0.00120 0.00586 0.00495

D106 3.12451 0.00016 0.00849 0.00237 0.01088 3.13539

D107 -3.13177 0.00006 0.00731 0.00032 0.00764 -3.12414

D108 -0.00636 0.00013 0.01116 0.00150 0.01266 0.00630

D109 0.00152 -0.00016 -0.00779 -0.00201 -0.00980 -0.00828

D110 3.05496 0.00012 -0.00084 0.00432 0.00349 3.05845

D111 -3.12391 -0.00023 -0.01164 -0.00318 -0.01483 -3.13874

D112 -0.07047 0.00005 -0.00468 0.00315 -0.00154 -0.07200

D113 -3.08808 0.00010 0.00853 0.00049 0.00902 -3.07906

D114 0.05165 0.00011 0.00769 0.00102 0.00872 0.06037

D115 0.03402 0.00018 0.01316 0.00191 0.01507 0.04909

D116 -3.10944 0.00019 0.01232 0.00243 0.01477 -3.09467

D117 1.13967 -0.00010 -0.02844 0.00210 -0.02634 1.11333

D118 -2.00131 -0.00009 -0.02821 0.00267 -0.02554 -2.02685

D119 -2.00022 -0.00011 -0.02768 0.00162 -0.02605 -2.02628

D120 1.14198 -0.00010 -0.02744 0.00219 -0.02525 1.11673

D121 3.13697 -0.00000 -0.00015 0.00042 0.00028 3.13725

D122 -0.00984 -0.00000 -0.00187 0.00023 -0.00164 -0.01148

D123 -0.00510 -0.00002 -0.00079 0.00006 -0.00073 -0.00583

D124 3.13127 -0.00002 -0.00252 -0.00013 -0.00265 3.12862

D125 -3.13480 -0.00004 -0.00046 -0.00098 -0.00144 -3.13624

D126 -0.00121 -0.00002 -0.00165 -0.00044 -0.00209 -0.00330

D127 0.00727 -0.00003 0.00018 -0.00062 -0.00044 0.00683

D128 3.14086 -0.00001 -0.00100 -0.00008 -0.00108 3.13978

D129 0.00079 0.00004 0.00082 0.00042 0.00124 0.00204

D130 3.13827 0.00002 -0.00006 0.00016 0.00010 3.13837

D131 -3.13554 0.00004 0.00255 0.00062 0.00317 -3.13237

D132 0.00193 0.00002 0.00167 0.00035 0.00203 0.00396

D133 0.00147 -0.00002 -0.00021 -0.00036 -0.00057 0.00090

D134 -3.14063 -0.00003 -0.00057 -0.00032 -0.00089 -3.14151

D135 -3.13599 0.00000 0.00067 -0.00009 0.00058 -3.13540

D136 0.00510 -0.00000 0.00032 -0.00006 0.00026 0.00537

D137 0.00069 -0.00002 -0.00040 -0.00019 -0.00060 0.00009

D138 -3.13713 -0.00001 0.00002 -0.00009 -0.00007 -3.13720

D139 -3.14041 -0.00002 -0.00005 -0.00023 -0.00028 -3.14068

D140 0.00497 -0.00000 0.00037 -0.00013 0.00025 0.00521

D141 -0.00514 0.00005 0.00041 0.00069 0.00110 -0.00404

D142 -3.13868 0.00003 0.00160 0.00015 0.00175 -3.13693

D143 3.13268 0.00003 -0.00001 0.00059 0.00058 3.13327

D144 -0.00086 0.00001 0.00118 0.00005 0.00123 0.00037

D145 -0.00147 0.00002 0.00021 0.00036 0.00057 -0.00090

D146 3.13599 -0.00000 -0.00067 0.00009 -0.00058 3.13540

D147 3.14063 0.00003 0.00057 0.00032 0.00089 3.14151

D148 -0.00510 0.00000 -0.00032 0.00006 -0.00026 -0.00537

D149 -0.00069 0.00002 0.00040 0.00019 0.00060 -0.00009

D150 3.13713 0.00001 -0.00002 0.00009 0.00007 3.13720

D151 3.14041 0.00002 0.00005 0.00023 0.00028 3.14068

D152 -0.00497 0.00000 -0.00037 0.00013 -0.00025 -0.00521

D153 -0.00079 -0.00004 -0.00082 -0.00042 -0.00124 -0.00204

D154 3.13554 -0.00004 -0.00255 -0.00062 -0.00317 3.13237

D155 -3.13827 -0.00002 0.00006 -0.00016 -0.00010 -3.13837

D156 -0.00193 -0.00002 -0.00167 -0.00035 -0.00203 -0.00396

D157 -3.13697 0.00000 0.00015 -0.00042 -0.00028 -3.13725

D158 0.00510 0.00002 0.00079 -0.00006 0.00073 0.00583

D159 0.00984 0.00000 0.00187 -0.00023 0.00164 0.01148

D160 -3.13127 0.00002 0.00252 0.00013 0.00265 -3.12862

D161 3.13480 0.00004 0.00046 0.00098 0.00144 3.13624

D162 0.00121 0.00002 0.00165 0.00044 0.00209 0.00330

D163 -0.00727 0.00003 -0.00018 0.00062 0.00044 -0.00683

D164 -3.14086 0.00001 0.00100 0.00008 0.00108 -3.13978

D165 0.00514 -0.00005 -0.00041 -0.00069 -0.00110 0.00404

D166 -3.13268 -0.00003 0.00001 -0.00059 -0.00058 -3.13327

D167 3.13868 -0.00003 -0.00160 -0.00015 -0.00175 3.13693

D168 0.00086 -0.00001 -0.00118 -0.00005 -0.00123 -0.00037

D169 3.13491 0.00004 0.00000 0.00122 0.00122 3.13613

D170 0.00120 0.00002 0.00147 0.00047 0.00194 0.00315

D171 -0.00728 0.00003 -0.00022 0.00067 0.00044 -0.00683

D172 -3.14098 0.00001 0.00124 -0.00008 0.00116 -3.13982

D173 -3.13727 0.00001 0.00065 -0.00047 0.00018 -3.13709

D174 0.00917 0.00001 0.00261 -0.00026 0.00235 0.01152

D175 0.00492 0.00002 0.00088 0.00009 0.00097 0.00588

D176 -3.13183 0.00003 0.00284 0.00030 0.00314 -3.12869

D177 0.00534 -0.00005 -0.00044 -0.00089 -0.00134 0.00400

D178 -3.13269 -0.00003 0.00010 -0.00069 -0.00059 -3.13328

D179 3.13900 -0.00003 -0.00191 -0.00015 -0.00206 3.13693

D180 0.00097 -0.00001 -0.00138 0.00006 -0.00132 -0.00034

D181 -0.00088 0.00003 0.00047 0.00035 0.00082 -0.00006

D182 3.14032 0.00002 0.00009 0.00029 0.00038 3.14070

D183 3.13713 0.00001 -0.00007 0.00015 0.00008 3.13720

D184 -0.00485 -0.00000 -0.00045 0.00008 -0.00037 -0.00522

D185 -0.00146 0.00002 0.00018 0.00039 0.00057 -0.00088

D186 3.13625 -0.00001 -0.00080 -0.00005 -0.00084 3.13541

D187 3.14052 0.00003 0.00056 0.00046 0.00102 3.14154

D188 -0.00496 -0.00000 -0.00042 0.00002 -0.00040 -0.00536

D189 -0.00061 -0.00005 -0.00087 -0.00062 -0.00149 -0.00210

D190 3.13611 -0.00005 -0.00284 -0.00083 -0.00367 3.13244

D191 -3.13834 -0.00002 0.00011 -0.00018 -0.00007 -3.13841

D192 -0.00162 -0.00002 -0.00187 -0.00039 -0.00226 -0.00387

D193 -3.13491 -0.00004 -0.00000 -0.00122 -0.00122 -3.13613

D194 -0.00120 -0.00002 -0.00147 -0.00047 -0.00194 -0.00315

D195 0.00728 -0.00003 0.00022 -0.00067 -0.00044 0.00683

D196 3.14098 -0.00001 -0.00124 0.00008 -0.00116 3.13982

D197 3.13727 -0.00001 -0.00065 0.00047 -0.00018 3.13709

D198 -0.00917 -0.00001 -0.00261 0.00026 -0.00235 -0.01152

D199 -0.00492 -0.00002 -0.00088 -0.00009 -0.00097 -0.00588

D200 3.13183 -0.00003 -0.00284 -0.00030 -0.00314 3.12869

D201 -0.00534 0.00005 0.00044 0.00089 0.00134 -0.00400

D202 3.13269 0.00003 -0.00010 0.00069 0.00059 3.13328

D203 -3.13900 0.00003 0.00191 0.00015 0.00206 -3.13693

D204 -0.00097 0.00001 0.00138 -0.00006 0.00132 0.00034

D205 0.00088 -0.00003 -0.00047 -0.00035 -0.00082 0.00006

D206 -3.14032 -0.00002 -0.00009 -0.00029 -0.00038 -3.14070

D207 -3.13713 -0.00001 0.00007 -0.00015 -0.00008 -3.13720

D208 0.00485 0.00000 0.00045 -0.00008 0.00037 0.00522

D209 0.00146 -0.00002 -0.00018 -0.00039 -0.00057 0.00088

D210 -3.13625 0.00001 0.00080 0.00005 0.00084 -3.13541

D211 -3.14052 -0.00003 -0.00056 -0.00046 -0.00102 -3.14154

D212 0.00496 0.00000 0.00042 -0.00002 0.00040 0.00536

D213 0.00061 0.00005 0.00087 0.00062 0.00149 0.00210

D214 -3.13611 0.00005 0.00284 0.00083 0.00367 -3.13244

D215 3.13834 0.00002 -0.00011 0.00018 0.00007 3.13841

D216 0.00162 0.00002 0.00187 0.00039 0.00226 0.00387

Item Value Threshold Converged?

Maximum Force 0.000406 0.000450 YES

RMS Force 0.000107 0.000300 YES

Maximum Displacement 0.159603 0.001800 NO

RMS Displacement 0.045098 0.001200 NO

Predicted change in Energy=-5.065967D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Aug 18 14:38:24 2019, MaxMem= 2013265920 cpu: 1.4

(Enter /home/kira/g09/l202.exe)

Stoichiometry C44H30N4(1-,2)

Framework group CS[SG(H2N2),X(C44H28N2)]

Deg. of freedom 116

Full point group CS NOp 2

RotChk: IX=3 Diff= 1.65D-04

Largest Abelian subgroup CS NOp 2

Largest concise Abelian subgroup CS NOp 2

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 4.258302 -0.148018 0.680975

2 6 0 2.898189 -0.007207 1.142064

3 7 0 2.117167 0.067647 -0.000000

4 6 0 2.898189 -0.007207 -1.142064

5 6 0 4.258302 -0.148018 -0.680975

6 6 0 2.460727 0.031300 -2.456420

7 6 0 1.095270 0.100448 -2.877988

8 7 0 0.000058 0.007505 -2.056380

9 6 0 -1.095200 0.100587 -2.877941

10 6 0 -0.687976 0.281389 -4.244202

11 6 0 0.688034 0.281348 -4.244238

12 6 0 2.460727 0.031300 2.456420

13 6 0 1.095270 0.100448 2.877988

14 6 0 0.688034 0.281348 4.244238

15 6 0 -0.687976 0.281389 4.244202

16 6 0 -1.095200 0.100587 2.877941

17 7 0 0.000058 0.007505 2.056380

18 6 0 -2.460651 0.031441 2.456403

19 6 0 -2.898156 -0.007168 1.142054

20 6 0 -4.258204 -0.148613 0.680986

21 6 0 -4.258204 -0.148613 -0.680986

22 6 0 -2.898156 -0.007168 -1.142054

23 7 0 -2.117190 0.067419 0.000000

24 6 0 -2.460651 0.031441 -2.456403

25 6 0 3.505476 -0.005148 -3.521500

26 6 0 4.438598 1.030812 -3.655320

27 6 0 5.415556 0.989155 -4.648750

28 6 0 5.474562 -0.090161 -5.528501

29 6 0 4.548782 -1.126909 -5.408170

30 6 0 3.573109 -1.082466 -4.415786

31 6 0 5.474562 -0.090161 5.528501

32 6 0 5.415556 0.989155 4.648750

33 6 0 4.438598 1.030812 3.655320

34 6 0 3.505476 -0.005148 3.521500

35 6 0 3.573109 -1.082466 4.415786

36 6 0 4.548782 -1.126909 5.408170

37 6 0 -3.505426 -0.004987 -3.521448

38 6 0 -3.572917 -1.082200 -4.415867

39 6 0 -4.548689 -1.126716 -5.408153

40 6 0 -5.474732 -0.090168 -5.528211

41 6 0 -5.415871 0.989037 -4.648316

42 6 0 -4.438777 1.030795 -3.655020

43 6 0 -3.505426 -0.004987 3.521448

44 6 0 -3.572917 -1.082200 4.415867

45 6 0 -4.548689 -1.126716 5.408153

46 6 0 -5.474732 -0.090168 5.528211

47 6 0 -5.415871 0.989037 4.648316

48 6 0 -4.438777 1.030795 3.655020

49 1 0 5.115842 -0.247715 1.327629

50 1 0 5.115842 -0.247715 -1.327629

51 1 0 -1.342100 0.406022 -5.094479

52 1 0 1.342116 0.405935 -5.094554

53 1 0 1.342116 0.405935 5.094554

54 1 0 -1.342100 0.406022 5.094479

55 1 0 -5.115640 -0.248959 1.327683

56 1 0 -5.115640 -0.248959 -1.327683

57 1 0 4.392024 1.877436 -2.978800

58 1 0 6.127352 1.803597 -4.737342

59 1 0 6.234649 -0.123701 -6.302143

60 1 0 4.588922 -1.973709 -6.085770

61 1 0 2.858655 -1.893271 -4.324084

62 1 0 6.234649 -0.123701 6.302143

63 1 0 6.127352 1.803597 4.737342

64 1 0 4.392024 1.877436 2.978800

65 1 0 2.858655 -1.893271 4.324084

66 1 0 4.588922 -1.973709 6.085770

67 1 0 -2.858250 -1.892843 -4.324370

68 1 0 -4.588714 -1.973428 -6.085869

69 1 0 -6.234907 -0.123775 -6.301763

70 1 0 -6.127875 1.803318 -4.736702

71 1 0 -4.392346 1.877301 -2.978339

72 1 0 -2.858250 -1.892843 4.324370

73 1 0 -4.588714 -1.973428 6.085869

74 1 0 -6.234907 -0.123775 6.301763

75 1 0 -6.127875 1.803318 4.736702

76 1 0 -4.392346 1.877301 2.978339

77 1 0 1.106889 0.097146 -0.000000

78 1 0 -1.107073 0.101246 0.000000

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

Rotational constants (GHZ): 0.0583822 0.0578365 0.0300188

Leave Link 202 at Sun Aug 18 14:38:24 2019, MaxMem= 2013265920 cpu: 0.1

(Enter /home/kira/g09/l301.exe)

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

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

There are 513 symmetry adapted cartesian basis functions of A' symmetry.

There are 489 symmetry adapted cartesian basis functions of A" symmetry.

There are 488 symmetry adapted basis functions of A' symmetry.

There are 466 symmetry adapted basis functions of A" symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 161 beta electrons

nuclear repulsion energy 5346.4317190988 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= 78 NActive= 78 NUniq= 41 SFac= 3.62D+00 NAtFMM= 60 NAOKFM=T 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= -0.2117082755 Hartrees.

Nuclear repulsion after empirical dispersion term = 5346.2200108233 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= 78.

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

Smoothing algorithm: York/Karplus (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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5706

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.25D-08

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 272

GePol: Fraction of low-weight points (<1% of avg) = 4.77%

GePol: Cavity surface area = 617.577 Ang\*\*2

GePol: Cavity volume = 628.966 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0019918773 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5346.2180189460 Hartrees.

Leave Link 301 at Sun Aug 18 14:38:24 2019, MaxMem= 2013265920 cpu: 1.0

(Enter /home/kira/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.

One-electron integral symmetry used in STVInt

NBasis= 954 RedAO= T EigKep= 9.01D-05 NBF= 488 466

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 488 466

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= 938 938 939 939 940 MxSgAt= 78 MxSgA2= 78.

Leave Link 302 at Sun Aug 18 14:38:25 2019, MaxMem= 2013265920 cpu: 10.7

(Enter /home/kira/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sun Aug 18 14:38:25 2019, MaxMem= 2013265920 cpu: 1.3

(Enter /home/kira/g09/l401.exe)

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

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000000 0.000000 -0.000034 Ang= -0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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The electronic state of the initial guess is 2-A'.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7586 S= 0.5043

Generating alternative initial guess.

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2000

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= -1914.57989132148

Leave Link 401 at Sun Aug 18 14:38:32 2019, MaxMem= 2013265920 cpu: 49.9

(Enter /home/kira/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3047318 IEndB= 3047318 NGot= 2013265920 MDV= 2011240249

LenX= 2011240249 LenY= 2010235243

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= 480000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 97675308.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.33D-15 for 5696.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.10D-15 for 2880 2681.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.11D-15 for 5696.

Iteration 1 A^-1\*A deviation from orthogonality is 1.03D-11 for 5000 4980.

E= -1914.47768147253

DIIS: error= 4.15D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.47768147253 IErMin= 1 ErrMin= 4.15D-03

ErrMax= 4.15D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.96D-02 BMatP= 2.96D-02

IDIUse=3 WtCom= 9.58D-01 WtEn= 4.15D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.446 Goal= None Shift= 0.000

Gap= 0.504 Goal= None Shift= 0.000

GapD= 0.446 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=1.21D-04 MaxDP=3.11D-03 OVMax= 2.07D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.21D-04 CP: 9.99D-01

E= -1914.49334554838 Delta-E= -0.015664075852 Rises=F Damp=F

DIIS: error= 5.61D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.49334554838 IErMin= 2 ErrMin= 5.61D-04

ErrMax= 5.61D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.00D-04 BMatP= 2.96D-02

IDIUse=3 WtCom= 9.94D-01 WtEn= 5.61D-03

Coeff-Com: -0.722D-01 0.107D+01

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

Coeff: -0.718D-01 0.107D+01

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=2.18D-05 MaxDP=5.46D-04 DE=-1.57D-02 OVMax= 3.19D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.91D-05 CP: 9.99D-01 1.09D+00

E= -1914.49360309308 Delta-E= -0.000257544696 Rises=F Damp=F

DIIS: error= 1.00D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.49360309308 IErMin= 3 ErrMin= 1.00D-04

ErrMax= 1.00D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.94D-05 BMatP= 4.00D-04

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.00D-03

Coeff-Com: -0.215D-01 0.243D+00 0.778D+00

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

Coeff: -0.214D-01 0.243D+00 0.779D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=5.78D-06 MaxDP=2.04D-04 DE=-2.58D-04 OVMax= 1.08D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 5.00D-06 CP: 9.99D-01 1.10D+00 8.89D-01

E= -1914.49361110545 Delta-E= -0.000008012371 Rises=F Damp=F

DIIS: error= 7.14D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.49361110545 IErMin= 4 ErrMin= 7.14D-05

ErrMax= 7.14D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.30D-05 BMatP= 3.94D-05

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

Coeff-Com: -0.590D-02 0.495D-01 0.368D+00 0.588D+00

Coeff: -0.590D-02 0.495D-01 0.368D+00 0.588D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=2.40D-06 MaxDP=1.31D-04 DE=-8.01D-06 OVMax= 6.37D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.92D-06 CP: 9.99D-01 1.11D+00 9.24D-01 7.48D-01

E= -1914.49361405106 Delta-E= -0.000002945608 Rises=F Damp=F

DIIS: error= 2.99D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.49361405106 IErMin= 5 ErrMin= 2.99D-05

ErrMax= 2.99D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.10D-06 BMatP= 1.30D-05

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

Coeff-Com: 0.794D-03-0.203D-01 0.453D-01 0.310D+00 0.665D+00

Coeff: 0.794D-03-0.203D-01 0.453D-01 0.310D+00 0.665D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=9.63D-07 MaxDP=4.93D-05 DE=-2.95D-06 OVMax= 2.30D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 4.87D-07 CP: 9.99D-01 1.11D+00 9.41D-01 8.20D-01 6.51D-01

E= -1914.49361454677 Delta-E= -0.000000495707 Rises=F Damp=F

DIIS: error= 8.00D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.49361454677 IErMin= 6 ErrMin= 8.00D-06

ErrMax= 8.00D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.25D-07 BMatP= 2.10D-06

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

Coeff-Com: 0.728D-03-0.142D-01 0.102D-01 0.159D+00 0.396D+00 0.449D+00

Coeff: 0.728D-03-0.142D-01 0.102D-01 0.159D+00 0.396D+00 0.449D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=2.89D-07 MaxDP=1.48D-05 DE=-4.96D-07 OVMax= 5.33D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.49D-07 CP: 9.99D-01 1.11D+00 9.44D-01 8.20D-01 6.86D-01

CP: 5.28D-01

E= -1914.49361460176 Delta-E= -0.000000054994 Rises=F Damp=F

DIIS: error= 1.59D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.49361460176 IErMin= 7 ErrMin= 1.59D-06

ErrMax= 1.59D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.14D-09 BMatP= 2.25D-07

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

Coeff-Com: 0.200D-03-0.351D-02-0.164D-03 0.343D-01 0.934D-01 0.158D+00

Coeff-Com: 0.717D+00

Coeff: 0.200D-03-0.351D-02-0.164D-03 0.343D-01 0.934D-01 0.158D+00

Coeff: 0.717D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=7.28D-08 MaxDP=4.28D-06 DE=-5.50D-08 OVMax= 1.33D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 6.51D-08 CP: 9.99D-01 1.11D+00 9.44D-01 8.22D-01 6.84D-01

CP: 5.87D-01 9.60D-01

E= -1914.49361460314 Delta-E= -0.000000001379 Rises=F Damp=F

DIIS: error= 1.41D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.49361460314 IErMin= 8 ErrMin= 1.41D-06

ErrMax= 1.41D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.94D-09 BMatP= 5.14D-09

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

Coeff-Com: -0.444D-04 0.115D-02-0.267D-02-0.156D-01-0.340D-01-0.514D-02

Coeff-Com: 0.465D+00 0.591D+00

Coeff: -0.444D-04 0.115D-02-0.267D-02-0.156D-01-0.340D-01-0.514D-02

Coeff: 0.465D+00 0.591D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=4.17D-08 MaxDP=2.20D-06 DE=-1.38D-09 OVMax= 1.01D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.63D-08 CP: 9.99D-01 1.11D+00 9.44D-01 8.22D-01 6.86D-01

CP: 5.91D-01 1.13D+00 7.02D-01

E= -1914.49361460429 Delta-E= -0.000000001148 Rises=F Damp=F

DIIS: error= 7.48D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.49361460429 IErMin= 9 ErrMin= 7.48D-07

ErrMax= 7.48D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.51D-10 BMatP= 2.94D-09

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

Coeff-Com: -0.429D-04 0.903D-03-0.104D-02-0.105D-01-0.256D-01-0.218D-01

Coeff-Com: 0.104D+00 0.242D+00 0.712D+00

Coeff: -0.429D-04 0.903D-03-0.104D-02-0.105D-01-0.256D-01-0.218D-01

Coeff: 0.104D+00 0.242D+00 0.712D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=1.89D-08 MaxDP=1.16D-06 DE=-1.15D-09 OVMax= 6.26D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.31D-08 CP: 9.99D-01 1.11D+00 9.44D-01 8.22D-01 6.87D-01

CP: 6.05D-01 1.15D+00 8.44D-01 1.22D+00

E= -1914.49361460466 Delta-E= -0.000000000371 Rises=F Damp=F

DIIS: error= 5.04D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.49361460466 IErMin=10 ErrMin= 5.04D-07

ErrMax= 5.04D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.62D-10 BMatP= 3.51D-10

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

Coeff-Com: 0.101D-04-0.386D-03 0.153D-02 0.618D-02 0.116D-01-0.862D-02

Coeff-Com: -0.298D+00-0.320D+00 0.418D+00 0.119D+01

Coeff: 0.101D-04-0.386D-03 0.153D-02 0.618D-02 0.116D-01-0.862D-02

Coeff: -0.298D+00-0.320D+00 0.418D+00 0.119D+01

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=2.67D-08 MaxDP=9.83D-07 DE=-3.71D-10 OVMax= 9.04D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 8.76D-09 CP: 9.99D-01 1.11D+00 9.44D-01 8.22D-01 6.87D-01

CP: 6.07D-01 1.23D+00 9.67D-01 2.00D+00 1.41D+00

E= -1914.49361460491 Delta-E= -0.000000000253 Rises=F Damp=F

DIIS: error= 1.33D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.49361460491 IErMin=11 ErrMin= 1.33D-07

ErrMax= 1.33D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.71D-11 BMatP= 1.62D-10

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

Coeff-Com: 0.110D-04-0.310D-03 0.834D-03 0.434D-02 0.906D-02-0.262D-03

Coeff-Com: -0.150D+00-0.181D+00 0.657D-01 0.529D+00 0.722D+00

Coeff: 0.110D-04-0.310D-03 0.834D-03 0.434D-02 0.906D-02-0.262D-03

Coeff: -0.150D+00-0.181D+00 0.657D-01 0.529D+00 0.722D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=7.82D-09 MaxDP=2.86D-07 DE=-2.53D-10 OVMax= 2.48D-06

Error on total polarization charges = 0.08606

SCF Done: E(UB3LYP) = -1914.49361460 A.U. after 11 cycles

NFock= 11 Conv=0.78D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7586 S= 0.5043

<L.S>= 0.000000000000E+00

KE= 1.906564641183D+03 PE=-1.517736946907D+04 EE= 6.010093194339D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.25

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7586, after 0.7500

Leave Link 502 at Sun Aug 18 14:44:39 2019, MaxMem= 2013265920 cpu: 2919.2

(Enter /home/kira/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 = 183

Leave Link 701 at Sun Aug 18 14:44:54 2019, MaxMem= 2013265920 cpu: 124.9

(Enter /home/kira/g09/l702.exe)

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

Leave Link 702 at Sun Aug 18 14:44:54 2019, MaxMem= 2013265920 cpu: 0.1

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 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= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

Petite list used in FoFCou.

Leave Link 703 at Sun Aug 18 14:45:59 2019, MaxMem= 2013265920 cpu: 517.5

(Enter /home/kira/g09/l716.exe)

Dipole =-4.86341600D-04-1.21283877D-01 1.18127730D-13

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000066727 0.000093086 -0.000056339

2 6 -0.000134725 0.000012179 0.000217175

3 7 0.000011547 -0.000324913 0.000000000

4 6 -0.000134725 0.000012179 -0.000217175

5 6 0.000066727 0.000093086 0.000056339

6 6 -0.000066301 0.000038694 0.000115229

7 6 0.000138554 -0.000007209 0.000035357

8 7 -0.000008835 0.000127480 0.000058690

9 6 -0.000127761 -0.000023978 0.000029528

10 6 0.000003901 -0.000017444 -0.000008708

11 6 -0.000008602 -0.000031325 -0.000000042

12 6 -0.000066301 0.000038694 -0.000115229

13 6 0.000138554 -0.000007209 -0.000035357

14 6 -0.000008602 -0.000031325 0.000000042

15 6 0.000003901 -0.000017444 0.000008708

16 6 -0.000127761 -0.000023978 -0.000029528

17 7 -0.000008835 0.000127480 -0.000058690

18 6 0.000060283 0.000054638 -0.000116897

19 6 0.000135222 -0.000015132 0.000221251

20 6 -0.000074096 0.000089664 -0.000068883

21 6 -0.000074096 0.000089664 0.000068883

22 6 0.000135222 -0.000015132 -0.000221251

23 7 0.000000118 -0.000238175 -0.000000000

24 6 0.000060283 0.000054638 0.000116897

25 6 0.000008872 -0.000068758 -0.000089081

26 6 -0.000023468 -0.000019095 -0.000029113

27 6 -0.000026862 0.000035430 -0.000005108

28 6 0.000004545 -0.000028735 -0.000005626

29 6 0.000023349 -0.000008476 0.000005361

30 6 0.000040515 0.000061544 0.000025596

31 6 0.000004545 -0.000028735 0.000005626

32 6 -0.000026862 0.000035430 0.000005108

33 6 -0.000023468 -0.000019095 0.000029113

34 6 0.000008872 -0.000068758 0.000089081

35 6 0.000040515 0.000061544 -0.000025596

36 6 0.000023349 -0.000008476 -0.000005361

37 6 -0.000002637 -0.000069545 -0.000086441

38 6 -0.000042106 0.000062091 0.000016424

39 6 -0.000022859 -0.000009006 0.000008794

40 6 -0.000003568 -0.000029592 -0.000007448

41 6 0.000030678 0.000037279 -0.000005378

42 6 0.000014838 -0.000021675 -0.000024962

43 6 -0.000002637 -0.000069545 0.000086441

44 6 -0.000042106 0.000062091 -0.000016424

45 6 -0.000022859 -0.000009006 -0.000008794

46 6 -0.000003568 -0.000029592 0.000007448

47 6 0.000030678 0.000037279 0.000005378

48 6 0.000014838 -0.000021675 0.000024962

49 1 0.000001673 -0.000030779 -0.000019605

50 1 0.000001673 -0.000030779 0.000019605

51 1 0.000011391 0.000002552 -0.000014806

52 1 -0.000008896 -0.000000402 -0.000014055

53 1 -0.000008896 -0.000000402 0.000014055

54 1 0.000011391 0.000002552 0.000014806

55 1 -0.000001687 -0.000031067 -0.000024422

56 1 -0.000001687 -0.000031067 0.000024422

57 1 -0.000005627 0.000001500 0.000013505

58 1 0.000004337 0.000002649 -0.000000666

59 1 0.000000893 -0.000001156 -0.000003412

60 1 0.000001696 -0.000004478 -0.000001827

61 1 -0.000010657 -0.000013356 0.000008978

62 1 0.000000893 -0.000001156 0.000003412

63 1 0.000004337 0.000002649 0.000000666

64 1 -0.000005627 0.000001500 -0.000013505

65 1 -0.000010657 -0.000013356 -0.000008978

66 1 0.000001696 -0.000004478 0.000001827

67 1 0.000007459 -0.000013782 0.000009976

68 1 -0.000002007 -0.000004449 -0.000002046

69 1 -0.000001380 -0.000001472 -0.000003401

70 1 -0.000004295 0.000003113 -0.000000419

71 1 0.000007045 0.000002110 0.000010237

72 1 0.000007459 -0.000013782 -0.000009976

73 1 -0.000002007 -0.000004449 0.000002046

74 1 -0.000001380 -0.000001472 0.000003401

75 1 -0.000004295 0.000003113 0.000000419

76 1 0.000007045 0.000002110 -0.000010237

77 1 0.000054820 0.000137964 0.000000000

78 1 -0.000037703 0.000078921 -0.000000000

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

Cartesian Forces: Max 0.000324913 RMS 0.000059549

Leave Link 716 at Sun Aug 18 14:45:59 2019, MaxMem= 2013265920 cpu: 0.2

(Enter /home/kira/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 0.000090526 RMS 0.000031745

Search for a local minimum.

Step number 7 out of a maximum of 452

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

RMS Force = .31745D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 2 3 4 5 6

7

DE= -4.91D-05 DEPred=-5.07D-05 R= 9.70D-01

TightC=F SS= 1.41D+00 RLast= 1.48D-01 DXNew= 1.6128D+00 4.4285D-01

Trust test= 9.70D-01 RLast= 1.48D-01 DXMaxT set to 9.59D-01

ITU= 1 0 1 1 1 1 0

Eigenvalues --- 0.00676 0.00983 0.00988 0.00990 0.01412

Eigenvalues --- 0.01605 0.01616 0.01623 0.01629 0.01637

Eigenvalues --- 0.01659 0.01723 0.01723 0.01723 0.01728

Eigenvalues --- 0.01737 0.01751 0.01774 0.01786 0.01792

Eigenvalues --- 0.01837 0.01848 0.01854 0.01856 0.01891

Eigenvalues --- 0.01902 0.01929 0.01943 0.01956 0.01986

Eigenvalues --- 0.02011 0.02020 0.02026 0.02027 0.02068

Eigenvalues --- 0.02068 0.02070 0.02071 0.02075 0.02087

Eigenvalues --- 0.02105 0.02115 0.02118 0.02119 0.02119

Eigenvalues --- 0.02130 0.02130 0.02132 0.02132 0.02132

Eigenvalues --- 0.02137 0.02160 0.02160 0.02160 0.02160

Eigenvalues --- 0.02162 0.02162 0.02162 0.02173 0.02173

Eigenvalues --- 0.02173 0.02173 0.02179 0.02181 0.02181

Eigenvalues --- 0.02181 0.02186 0.02186 0.02187 0.02187

Eigenvalues --- 0.02203 0.02216 0.02217 0.02280 0.03294

Eigenvalues --- 0.15903 0.15925 0.15935 0.15997 0.15997

Eigenvalues --- 0.15997 0.15998 0.15998 0.15999 0.15999

Eigenvalues --- 0.15999 0.15999 0.15999 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16004 0.16020 0.16108

Eigenvalues --- 0.21950 0.22000 0.22000 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22001 0.22552 0.22758

Eigenvalues --- 0.22773 0.22815 0.22834 0.23472 0.23472

Eigenvalues --- 0.23475 0.23541 0.23818 0.24413 0.24732

Eigenvalues --- 0.24832 0.24853 0.24969 0.24989 0.24997

Eigenvalues --- 0.24998 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25105

Eigenvalues --- 0.26089 0.27685 0.34159 0.34182 0.34206

Eigenvalues --- 0.34882 0.35413 0.35413 0.35413 0.35413

Eigenvalues --- 0.35415 0.35415 0.35416 0.35416 0.35416

Eigenvalues --- 0.35416 0.35416 0.35435 0.35506 0.35507

Eigenvalues --- 0.35508 0.35526 0.35542 0.35545 0.35547

Eigenvalues --- 0.35746 0.36056 0.36057 0.36058 0.36112

Eigenvalues --- 0.36249 0.36250 0.36251 0.36253 0.37118

Eigenvalues --- 0.37158 0.37262 0.37293 0.37933 0.39131

Eigenvalues --- 0.39744 0.39947 0.40259 0.40421 0.40463

Eigenvalues --- 0.40761 0.41782 0.41787 0.41798 0.42091

Eigenvalues --- 0.42091 0.42094 0.42095 0.42146 0.43148

Eigenvalues --- 0.43274 0.44660 0.45339 0.45569 0.45571

Eigenvalues --- 0.45586 0.45587 0.45703 0.45770 0.45854

Eigenvalues --- 0.45875 0.45930 0.45940 0.45942 0.45948

Eigenvalues --- 0.45969 0.46660 0.46660 0.46661 0.46666

Eigenvalues --- 0.47073 0.47079 0.47086 0.47523 0.48190

Eigenvalues --- 0.48278 0.48366 0.49336 0.49433 0.49974

Eigenvalues --- 0.50638 0.50809 0.54882

En-DIIS/RFO-DIIS IScMMF= 0 using points: 7 6 5 4 3

RFO step: Lambda=-2.29826491D-06.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 4.14D-04 SmlDif= 1.00D-05

RMS Error= 0.2123192818D-03 NUsed= 5 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.79869 0.21090 0.04849 0.00355 -0.06162

Iteration 1 RMS(Cart)= 0.01750092 RMS(Int)= 0.00007848

Iteration 2 RMS(Cart)= 0.00013548 RMS(Int)= 0.00000688

Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00000688

ITry= 1 IFail=0 DXMaxC= 6.27D-02 DCOld= 1.00D+10 DXMaxT= 9.59D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.58D-08 for atom 62.

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

(Linear) (Quad) (Total)

R1 2.72693 0.00008 0.00017 0.00001 0.00018 2.72711

R2 2.57371 -0.00001 -0.00019 0.00018 -0.00001 2.57370

R3 2.03834 -0.00001 0.00004 -0.00004 0.00000 2.03835

R4 2.61842 0.00003 -0.00004 0.00003 -0.00002 2.61840

R5 2.61875 -0.00009 -0.00019 -0.00012 -0.00030 2.61844

R6 2.61842 0.00003 -0.00004 0.00003 -0.00002 2.61840

R7 1.90996 -0.00005 0.00004 -0.00011 -0.00007 1.90990

R8 2.72693 0.00008 0.00017 0.00001 0.00018 2.72711

R9 2.61875 -0.00009 -0.00019 -0.00012 -0.00030 2.61844

R10 2.03834 -0.00001 0.00004 -0.00004 0.00000 2.03835

R11 2.70368 -0.00009 -0.00016 -0.00027 -0.00043 2.70325

R12 2.82021 0.00007 0.00035 0.00028 0.00062 2.82083

R13 2.59324 0.00006 -0.00022 0.00030 0.00008 2.59332

R14 2.71569 0.00001 0.00007 -0.00002 0.00006 2.71575

R15 2.59328 0.00005 -0.00020 0.00028 0.00007 2.59334

R16 2.71568 0.00002 0.00005 0.00002 0.00007 2.71575

R17 2.70365 -0.00009 -0.00023 -0.00020 -0.00043 2.70322

R18 2.60028 -0.00002 -0.00004 0.00006 0.00003 2.60031

R19 2.04089 0.00001 -0.00002 0.00000 -0.00002 2.04087

R20 2.04089 0.00001 -0.00004 0.00002 -0.00001 2.04087

R21 2.70368 -0.00009 -0.00016 -0.00027 -0.00043 2.70325

R22 2.82021 0.00007 0.00035 0.00028 0.00062 2.82083

R23 2.71569 0.00001 0.00007 -0.00002 0.00006 2.71575

R24 2.59324 0.00006 -0.00022 0.00030 0.00008 2.59332

R25 2.60028 -0.00002 -0.00004 0.00006 0.00003 2.60031

R26 2.04089 0.00001 -0.00004 0.00002 -0.00001 2.04087

R27 2.71568 0.00002 0.00005 0.00002 0.00007 2.71575

R28 2.04089 0.00001 -0.00002 0.00000 -0.00002 2.04087

R29 2.59328 0.00005 -0.00020 0.00028 0.00007 2.59334

R30 2.70365 -0.00009 -0.00023 -0.00020 -0.00043 2.70322

R31 2.61876 -0.00008 -0.00027 -0.00005 -0.00032 2.61844

R32 2.82019 0.00007 0.00036 0.00033 0.00069 2.82088

R33 2.72692 0.00009 0.00017 0.00002 0.00020 2.72712

R34 2.61832 0.00005 -0.00006 0.00010 0.00003 2.61835

R35 2.57375 -0.00002 -0.00018 0.00014 -0.00003 2.57372

R36 2.03835 -0.00001 0.00005 -0.00006 -0.00000 2.03835

R37 2.72692 0.00009 0.00017 0.00002 0.00020 2.72712

R38 2.03835 -0.00001 0.00005 -0.00006 -0.00000 2.03835

R39 2.61832 0.00005 -0.00006 0.00010 0.00003 2.61835

R40 2.61876 -0.00008 -0.00027 -0.00005 -0.00032 2.61844

R41 1.90991 -0.00003 0.00006 -0.00008 -0.00003 1.90989

R42 2.82019 0.00007 0.00036 0.00033 0.00069 2.82088

R43 2.64686 -0.00002 -0.00035 0.00004 -0.00031 2.64654

R44 2.64894 -0.00004 -0.00024 -0.00009 -0.00032 2.64862

R45 2.63418 0.00000 0.00010 -0.00001 0.00008 2.63426

R46 2.04983 0.00001 0.00005 0.00000 0.00005 2.04988

R47 2.63369 0.00002 -0.00001 0.00003 0.00002 2.63371

R48 2.05087 0.00000 -0.00002 0.00002 -0.00000 2.05087

R49 2.63642 -0.00001 -0.00000 -0.00003 -0.00003 2.63639

R50 2.05049 0.00000 -0.00001 0.00002 0.00001 2.05050

R51 2.63123 0.00001 0.00011 0.00002 0.00013 2.63136

R52 2.05087 0.00000 -0.00002 0.00002 -0.00000 2.05087

R53 2.04951 0.00002 0.00005 0.00003 0.00007 2.04959

R54 2.63369 0.00002 -0.00001 0.00003 0.00002 2.63371

R55 2.63642 -0.00001 -0.00000 -0.00003 -0.00003 2.63639

R56 2.05049 0.00000 -0.00001 0.00002 0.00001 2.05050

R57 2.63418 0.00000 0.00010 -0.00001 0.00008 2.63426

R58 2.05087 0.00000 -0.00002 0.00002 -0.00000 2.05087

R59 2.64686 -0.00002 -0.00035 0.00004 -0.00031 2.64654

R60 2.04983 0.00001 0.00005 0.00000 0.00005 2.04988

R61 2.64894 -0.00004 -0.00024 -0.00009 -0.00032 2.64862

R62 2.63123 0.00001 0.00011 0.00002 0.00013 2.63136

R63 2.04951 0.00002 0.00005 0.00003 0.00007 2.04959

R64 2.05087 0.00000 -0.00002 0.00002 -0.00000 2.05087

R65 2.64894 -0.00004 -0.00028 -0.00006 -0.00034 2.64860

R66 2.64685 -0.00002 -0.00039 0.00006 -0.00033 2.64652

R67 2.63123 0.00001 0.00012 0.00002 0.00014 2.63137

R68 2.04951 0.00002 0.00006 0.00001 0.00007 2.04959

R69 2.63642 -0.00001 -0.00000 -0.00004 -0.00004 2.63638

R70 2.05087 0.00000 -0.00002 0.00002 -0.00000 2.05087

R71 2.63369 0.00002 -0.00000 0.00002 0.00002 2.63371

R72 2.05049 0.00000 -0.00001 0.00002 0.00001 2.05050

R73 2.63418 -0.00000 0.00010 -0.00001 0.00009 2.63427

R74 2.05087 0.00001 -0.00002 0.00002 -0.00000 2.05087

R75 2.04983 0.00001 0.00006 -0.00001 0.00005 2.04988

R76 2.64894 -0.00004 -0.00028 -0.00006 -0.00034 2.64860

R77 2.64685 -0.00002 -0.00039 0.00006 -0.00033 2.64652

R78 2.63123 0.00001 0.00012 0.00002 0.00014 2.63137

R79 2.04951 0.00002 0.00006 0.00001 0.00007 2.04959

R80 2.63642 -0.00001 -0.00000 -0.00004 -0.00004 2.63638

R81 2.05087 0.00000 -0.00002 0.00002 -0.00000 2.05087

R82 2.63369 0.00002 -0.00000 0.00002 0.00002 2.63371

R83 2.05049 0.00000 -0.00001 0.00002 0.00001 2.05050

R84 2.63418 -0.00000 0.00010 -0.00001 0.00009 2.63427

R85 2.05087 0.00001 -0.00002 0.00002 -0.00000 2.05087

R86 2.04983 0.00001 0.00006 -0.00001 0.00005 2.04988

A1 1.89603 0.00002 -0.00001 0.00003 0.00002 1.89605

A2 2.17340 0.00001 -0.00019 0.00009 -0.00010 2.17330

A3 2.21368 -0.00003 0.00020 -0.00013 0.00007 2.21375

A4 1.84750 -0.00006 0.00004 -0.00014 -0.00011 1.84739

A5 2.21844 0.00005 -0.00018 -0.00003 -0.00018 2.21826

A6 2.21719 0.00001 0.00012 0.00017 0.00027 2.21746

A7 1.93769 0.00008 -0.00004 0.00021 0.00018 1.93787

A8 2.17123 -0.00004 -0.00010 0.00010 -0.00000 2.17123

A9 2.17123 -0.00004 -0.00010 0.00010 -0.00000 2.17123

A10 1.84750 -0.00006 0.00004 -0.00014 -0.00011 1.84739

A11 2.21719 0.00001 0.00012 0.00017 0.00027 2.21746

A12 2.21844 0.00005 -0.00018 -0.00003 -0.00018 2.21826

A13 1.89603 0.00002 -0.00001 0.00003 0.00002 1.89605

A14 2.21368 -0.00003 0.00020 -0.00013 0.00007 2.21375

A15 2.17340 0.00001 -0.00019 0.00009 -0.00010 2.17330

A16 2.19209 -0.00001 0.00070 -0.00007 0.00059 2.19268

A17 2.04342 0.00005 -0.00032 -0.00004 -0.00034 2.04308

A18 2.04768 -0.00004 -0.00038 0.00011 -0.00025 2.04742

A19 2.19198 0.00005 0.00015 0.00009 0.00021 2.19219

A20 2.16116 -0.00004 -0.00020 0.00002 -0.00016 2.16100

A21 1.93004 -0.00001 0.00006 -0.00011 -0.00006 1.92999

A22 1.84829 -0.00001 -0.00001 0.00008 0.00008 1.84836

A23 1.93002 -0.00001 0.00010 -0.00014 -0.00005 1.92997

A24 2.19204 0.00004 0.00015 0.00004 0.00017 2.19221

A25 2.16113 -0.00003 -0.00025 0.00010 -0.00012 2.16101

A26 1.85813 0.00001 -0.00009 0.00012 0.00002 1.85815

A27 2.20358 0.00001 -0.00005 0.00014 0.00009 2.20367

A28 2.22139 -0.00002 0.00014 -0.00026 -0.00011 2.22127

A29 1.85809 0.00002 -0.00004 0.00009 0.00004 1.85813

A30 2.20362 0.00001 -0.00007 0.00013 0.00006 2.20369

A31 2.22138 -0.00003 0.00012 -0.00022 -0.00011 2.22128

A32 2.19209 -0.00001 0.00070 -0.00007 0.00059 2.19268

A33 2.04342 0.00005 -0.00032 -0.00004 -0.00034 2.04308

A34 2.04768 -0.00004 -0.00038 0.00011 -0.00025 2.04742

A35 2.16116 -0.00004 -0.00020 0.00002 -0.00016 2.16100

A36 2.19198 0.00005 0.00015 0.00009 0.00021 2.19219

A37 1.93004 -0.00001 0.00006 -0.00011 -0.00006 1.92999

A38 1.85809 0.00002 -0.00004 0.00009 0.00004 1.85813

A39 2.20362 0.00001 -0.00007 0.00013 0.00006 2.20369

A40 2.22138 -0.00003 0.00012 -0.00022 -0.00011 2.22128

A41 1.85813 0.00001 -0.00009 0.00012 0.00002 1.85815

A42 2.22139 -0.00002 0.00014 -0.00026 -0.00011 2.22127

A43 2.20358 0.00001 -0.00005 0.00014 0.00009 2.20367

A44 1.93002 -0.00001 0.00010 -0.00014 -0.00005 1.92997

A45 2.16113 -0.00003 -0.00025 0.00010 -0.00012 2.16101

A46 2.19204 0.00004 0.00015 0.00004 0.00017 2.19221

A47 1.84829 -0.00001 -0.00001 0.00008 0.00008 1.84836

A48 2.19211 -0.00002 0.00074 -0.00011 0.00060 2.19271

A49 2.04772 -0.00004 -0.00046 0.00013 -0.00031 2.04742

A50 2.04335 0.00006 -0.00029 -0.00003 -0.00029 2.04306

A51 2.21846 0.00005 -0.00019 -0.00003 -0.00019 2.21828

A52 2.21720 0.00001 0.00008 0.00020 0.00026 2.21745

A53 1.84746 -0.00006 0.00009 -0.00017 -0.00009 1.84738

A54 1.89601 0.00003 -0.00003 0.00006 0.00003 1.89604

A55 2.17337 0.00001 -0.00016 0.00008 -0.00008 2.17329

A56 2.21373 -0.00004 0.00020 -0.00015 0.00005 2.21378

A57 1.89601 0.00003 -0.00003 0.00006 0.00003 1.89604

A58 2.21373 -0.00004 0.00020 -0.00015 0.00005 2.21378

A59 2.17337 0.00001 -0.00016 0.00008 -0.00008 2.17329

A60 1.84746 -0.00006 0.00009 -0.00017 -0.00009 1.84738

A61 2.21846 0.00005 -0.00019 -0.00003 -0.00019 2.21828

A62 2.21720 0.00001 0.00008 0.00020 0.00026 2.21745

A63 1.93778 0.00006 -0.00009 0.00021 0.00013 1.93791

A64 2.17139 -0.00003 -0.00010 0.00004 -0.00006 2.17134

A65 2.17139 -0.00003 -0.00010 0.00004 -0.00006 2.17134

A66 2.19211 -0.00002 0.00074 -0.00011 0.00060 2.19271

A67 2.04772 -0.00004 -0.00046 0.00013 -0.00031 2.04742

A68 2.04335 0.00006 -0.00029 -0.00003 -0.00029 2.04306

A69 2.11355 -0.00003 -0.00020 -0.00027 -0.00047 2.11308

A70 2.10349 0.00004 -0.00027 0.00036 0.00009 2.10357

A71 2.06615 -0.00001 0.00048 -0.00009 0.00039 2.06653

A72 2.10936 0.00001 -0.00024 0.00008 -0.00016 2.10920

A73 2.08184 -0.00002 0.00012 -0.00012 0.00000 2.08184

A74 2.09197 0.00000 0.00013 0.00003 0.00016 2.09213

A75 2.09750 -0.00001 -0.00003 -0.00006 -0.00008 2.09741

A76 2.08911 0.00000 -0.00001 0.00009 0.00007 2.08919

A77 2.09656 0.00000 0.00004 -0.00003 0.00001 2.09657

A78 2.08628 -0.00001 0.00010 0.00000 0.00011 2.08638

A79 2.09863 0.00001 -0.00005 0.00001 -0.00004 2.09859

A80 2.09828 0.00000 -0.00005 -0.00002 -0.00007 2.09821

A81 2.09756 -0.00001 -0.00007 -0.00001 -0.00008 2.09748

A82 2.09605 0.00000 0.00006 -0.00005 0.00001 2.09606

A83 2.08957 0.00000 0.00001 0.00006 0.00007 2.08964

A84 2.10952 0.00002 -0.00024 0.00007 -0.00017 2.10935

A85 2.08155 -0.00002 0.00014 -0.00012 0.00003 2.08157

A86 2.09209 -0.00000 0.00010 0.00005 0.00015 2.09224

A87 2.08628 -0.00001 0.00010 0.00000 0.00011 2.08638

A88 2.09863 0.00001 -0.00005 0.00001 -0.00004 2.09859

A89 2.09828 0.00000 -0.00005 -0.00002 -0.00007 2.09821

A90 2.09750 -0.00001 -0.00003 -0.00006 -0.00008 2.09741

A91 2.09656 0.00000 0.00004 -0.00003 0.00001 2.09657

A92 2.08911 0.00000 -0.00001 0.00009 0.00007 2.08919

A93 2.10936 0.00001 -0.00024 0.00008 -0.00016 2.10920

A94 2.09197 0.00000 0.00013 0.00003 0.00016 2.09213

A95 2.08184 -0.00002 0.00012 -0.00012 0.00000 2.08184

A96 2.11355 -0.00003 -0.00020 -0.00027 -0.00047 2.11308

A97 2.10349 0.00004 -0.00027 0.00036 0.00009 2.10357

A98 2.06615 -0.00001 0.00048 -0.00009 0.00039 2.06653

A99 2.10952 0.00002 -0.00024 0.00007 -0.00017 2.10935

A100 2.08155 -0.00002 0.00014 -0.00012 0.00003 2.08157

A101 2.09209 -0.00000 0.00010 0.00005 0.00015 2.09224

A102 2.09756 -0.00001 -0.00007 -0.00001 -0.00008 2.09748

A103 2.09605 0.00000 0.00006 -0.00005 0.00001 2.09606

A104 2.08957 0.00000 0.00001 0.00006 0.00007 2.08964

A105 2.10346 0.00004 -0.00030 0.00039 0.00009 2.10354

A106 2.11357 -0.00003 -0.00023 -0.00027 -0.00049 2.11308

A107 2.06616 -0.00002 0.00053 -0.00013 0.00040 2.06656

A108 2.10951 0.00002 -0.00026 0.00009 -0.00018 2.10933

A109 2.08155 -0.00002 0.00014 -0.00012 0.00002 2.08157

A110 2.09210 -0.00001 0.00012 0.00003 0.00015 2.09225

A111 2.09756 -0.00000 -0.00008 -0.00001 -0.00009 2.09747

A112 2.08957 0.00000 0.00001 0.00007 0.00008 2.08965

A113 2.09605 0.00000 0.00007 -0.00006 0.00001 2.09606

A114 2.08628 -0.00001 0.00011 0.00000 0.00011 2.08640

A115 2.09827 0.00000 -0.00006 -0.00001 -0.00007 2.09820

A116 2.09863 0.00001 -0.00005 0.00001 -0.00004 2.09859

A117 2.09749 -0.00001 -0.00003 -0.00005 -0.00009 2.09741

A118 2.09656 0.00000 0.00005 -0.00004 0.00001 2.09657

A119 2.08912 0.00000 -0.00002 0.00009 0.00008 2.08920

A120 2.10935 0.00002 -0.00027 0.00010 -0.00017 2.10918

A121 2.08183 -0.00002 0.00012 -0.00011 0.00000 2.08184

A122 2.09198 0.00000 0.00015 0.00001 0.00017 2.09215

A123 2.10346 0.00004 -0.00030 0.00039 0.00009 2.10354

A124 2.11357 -0.00003 -0.00023 -0.00027 -0.00049 2.11308

A125 2.06616 -0.00002 0.00053 -0.00013 0.00040 2.06656

A126 2.10951 0.00002 -0.00026 0.00009 -0.00018 2.10933

A127 2.08155 -0.00002 0.00014 -0.00012 0.00002 2.08157

A128 2.09210 -0.00001 0.00012 0.00003 0.00015 2.09225

A129 2.09756 -0.00000 -0.00008 -0.00001 -0.00009 2.09747

A130 2.08957 0.00000 0.00001 0.00007 0.00008 2.08965

A131 2.09605 0.00000 0.00007 -0.00006 0.00001 2.09606

A132 2.08628 -0.00001 0.00011 0.00000 0.00011 2.08640

A133 2.09827 0.00000 -0.00006 -0.00001 -0.00007 2.09820

A134 2.09863 0.00001 -0.00005 0.00001 -0.00004 2.09859

A135 2.09749 -0.00001 -0.00003 -0.00005 -0.00009 2.09741

A136 2.09656 0.00000 0.00005 -0.00004 0.00001 2.09657

A137 2.08912 0.00000 -0.00002 0.00009 0.00008 2.08920

A138 2.10935 0.00002 -0.00027 0.00010 -0.00017 2.10918

A139 2.08183 -0.00002 0.00012 -0.00011 0.00000 2.08184

A140 2.09198 0.00000 0.00015 0.00001 0.00017 2.09215

D1 0.00448 -0.00001 -0.00173 0.00084 -0.00089 0.00359

D2 3.13549 -0.00004 -0.00384 0.00080 -0.00304 3.13244

D3 -3.12489 0.00002 -0.00230 0.00165 -0.00064 -3.12553

D4 0.00611 -0.00000 -0.00441 0.00161 -0.00280 0.00332

D5 -0.00000 -0.00000 0.00000 0.00000 -0.00000 -0.00000

D6 -3.12901 0.00003 -0.00057 0.00083 0.00026 -3.12876

D7 3.12901 -0.00003 0.00057 -0.00083 -0.00026 3.12876

D8 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D9 -0.00750 0.00002 0.00290 -0.00141 0.00149 -0.00601

D10 3.05364 0.00004 -0.00016 0.00401 0.00385 3.05749

D11 -3.13852 0.00004 0.00501 -0.00137 0.00364 -3.13487

D12 -0.07737 0.00007 0.00195 0.00405 0.00600 -0.07137

D13 -3.07962 -0.00003 -0.00202 -0.00010 -0.00212 -3.08173

D14 0.05988 -0.00005 -0.00218 -0.00055 -0.00273 0.05716

D15 0.04922 -0.00006 -0.00456 -0.00015 -0.00472 0.04450

D16 -3.09447 -0.00008 -0.00472 -0.00060 -0.00533 -3.09979

D17 0.00750 -0.00002 -0.00290 0.00141 -0.00149 0.00601

D18 3.13852 -0.00004 -0.00501 0.00137 -0.00364 3.13487

D19 -3.05364 -0.00004 0.00016 -0.00401 -0.00385 -3.05749

D20 0.07737 -0.00007 -0.00195 -0.00405 -0.00600 0.07137

D21 -0.00448 0.00001 0.00173 -0.00084 0.00089 -0.00359

D22 3.12489 -0.00002 0.00230 -0.00165 0.00064 3.12553

D23 -3.13549 0.00004 0.00384 -0.00080 0.00304 -3.13244

D24 -0.00611 0.00000 0.00441 -0.00161 0.00280 -0.00332

D25 -0.04922 0.00006 0.00456 0.00015 0.00472 -0.04450

D26 3.09447 0.00008 0.00472 0.00060 0.00533 3.09979

D27 3.07962 0.00003 0.00202 0.00010 0.00212 3.08173

D28 -0.05988 0.00005 0.00218 0.00055 0.00273 -0.05716

D29 -0.11872 0.00007 0.00771 0.00140 0.00911 -0.10961

D30 3.02160 0.00005 0.00511 0.00239 0.00750 3.02910

D31 3.02078 0.00005 0.00754 0.00095 0.00849 3.02927

D32 -0.12209 0.00003 0.00495 0.00194 0.00689 -0.11520

D33 -1.11696 -0.00006 -0.00885 -0.00177 -0.01062 -1.12758

D34 2.02615 -0.00006 -0.00927 -0.00154 -0.01081 2.01534

D35 2.02655 -0.00005 -0.00870 -0.00136 -0.01006 2.01649

D36 -1.11352 -0.00005 -0.00912 -0.00113 -0.01025 -1.12378

D37 -3.12337 -0.00001 -0.00270 -0.00036 -0.00306 -3.12643

D38 0.01935 0.00000 -0.00039 -0.00124 -0.00163 0.01772

D39 3.13051 0.00002 0.00252 -0.00006 0.00246 3.13297

D40 -0.02478 0.00001 0.00272 -0.00020 0.00253 -0.02225

D41 -0.01219 -0.00000 0.00026 0.00080 0.00106 -0.01113

D42 3.11571 -0.00001 0.00047 0.00067 0.00113 3.11684

D43 -0.01932 -0.00001 0.00037 0.00122 0.00159 -0.01773

D44 3.12322 0.00002 0.00290 0.00036 0.00326 3.12648

D45 0.01210 0.00001 -0.00022 -0.00074 -0.00096 0.01114

D46 -3.11574 0.00001 -0.00044 -0.00065 -0.00110 -3.11683

D47 -3.13041 -0.00002 -0.00269 0.00009 -0.00259 -3.13301

D48 0.02493 -0.00001 -0.00291 0.00018 -0.00273 0.02220

D49 0.11876 -0.00008 -0.00797 -0.00141 -0.00938 0.10938

D50 -3.02066 -0.00006 -0.00792 -0.00101 -0.00893 -3.02960

D51 -3.02177 -0.00005 -0.00513 -0.00237 -0.00750 -3.02927

D52 0.12199 -0.00003 -0.00508 -0.00197 -0.00705 0.11494

D53 0.00005 -0.00000 -0.00003 -0.00003 -0.00006 -0.00001

D54 -3.12766 0.00000 -0.00023 0.00010 -0.00013 -3.12779

D55 3.12771 -0.00001 0.00020 -0.00012 0.00008 3.12779

D56 -0.00001 -0.00000 -0.00000 0.00001 0.00001 0.00000

D57 -3.02160 -0.00005 -0.00511 -0.00239 -0.00750 -3.02910

D58 0.11872 -0.00007 -0.00771 -0.00140 -0.00911 0.10961

D59 0.12209 -0.00003 -0.00495 -0.00194 -0.00689 0.11520

D60 -3.02078 -0.00005 -0.00754 -0.00095 -0.00849 -3.02927

D61 1.11696 0.00006 0.00885 0.00177 0.01062 1.12758

D62 -2.02615 0.00006 0.00927 0.00154 0.01081 -2.01534

D63 -2.02655 0.00005 0.00870 0.00136 0.01006 -2.01649

D64 1.11352 0.00005 0.00912 0.00113 0.01025 1.12378

D65 -3.13051 -0.00002 -0.00252 0.00006 -0.00246 -3.13297

D66 0.02478 -0.00001 -0.00272 0.00020 -0.00253 0.02225

D67 0.01219 0.00000 -0.00026 -0.00080 -0.00106 0.01113

D68 -3.11571 0.00001 -0.00047 -0.00067 -0.00113 -3.11684

D69 3.12337 0.00001 0.00270 0.00036 0.00306 3.12643

D70 -0.01935 -0.00000 0.00039 0.00124 0.00163 -0.01772

D71 -0.00005 0.00000 0.00003 0.00003 0.00006 0.00001

D72 -3.12771 0.00001 -0.00020 0.00012 -0.00008 -3.12779

D73 3.12766 -0.00000 0.00023 -0.00010 0.00013 3.12779

D74 0.00001 0.00000 0.00000 -0.00001 -0.00001 -0.00000

D75 -0.01210 -0.00001 0.00022 0.00074 0.00096 -0.01114

D76 3.13041 0.00002 0.00269 -0.00009 0.00259 3.13301

D77 3.11574 -0.00001 0.00044 0.00065 0.00110 3.11683

D78 -0.02493 0.00001 0.00291 -0.00018 0.00273 -0.02220

D79 0.01932 0.00001 -0.00037 -0.00122 -0.00159 0.01773

D80 -3.12322 -0.00002 -0.00290 -0.00036 -0.00326 -3.12648

D81 3.02177 0.00005 0.00513 0.00237 0.00750 3.02927

D82 -0.12199 0.00003 0.00508 0.00197 0.00705 -0.11494

D83 -0.11876 0.00008 0.00797 0.00141 0.00938 -0.10938

D84 3.02066 0.00006 0.00792 0.00101 0.00893 3.02960

D85 3.07906 0.00004 0.00296 0.00001 0.00297 3.08203

D86 -0.04909 0.00006 0.00496 0.00004 0.00500 -0.04409

D87 -0.06037 0.00005 0.00301 0.00041 0.00342 -0.05695

D88 3.09467 0.00008 0.00501 0.00044 0.00545 3.10012

D89 -1.11333 -0.00005 -0.01009 -0.00110 -0.01120 -1.12453

D90 2.02685 -0.00005 -0.00978 -0.00135 -0.01113 2.01571

D91 2.02628 -0.00006 -0.01013 -0.00147 -0.01161 2.01467

D92 -1.11673 -0.00006 -0.00982 -0.00172 -0.01154 -1.12827

D93 -3.13539 0.00003 0.00343 -0.00077 0.00266 -3.13273

D94 -0.00630 0.00000 0.00416 -0.00155 0.00260 -0.00370

D95 -0.00495 0.00001 0.00177 -0.00080 0.00097 -0.00398

D96 3.12414 -0.00002 0.00250 -0.00158 0.00092 3.12506

D97 3.13874 -0.00004 -0.00462 0.00131 -0.00331 3.13542

D98 0.07200 -0.00004 -0.00062 -0.00292 -0.00354 0.06846

D99 0.00828 -0.00002 -0.00296 0.00134 -0.00162 0.00666

D100 -3.05845 -0.00002 0.00104 -0.00289 -0.00185 -3.06030

D101 0.00000 -0.00000 -0.00000 0.00000 0.00000 0.00000

D102 3.12872 -0.00003 0.00074 -0.00080 -0.00006 3.12866

D103 -3.12872 0.00003 -0.00074 0.00080 0.00006 -3.12866

D104 -0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D105 0.00495 -0.00001 -0.00177 0.00080 -0.00097 0.00398

D106 3.13539 -0.00003 -0.00343 0.00077 -0.00266 3.13273

D107 -3.12414 0.00002 -0.00250 0.00158 -0.00092 -3.12506

D108 0.00630 -0.00000 -0.00416 0.00155 -0.00260 0.00370

D109 -0.00828 0.00002 0.00296 -0.00134 0.00162 -0.00666

D110 3.05845 0.00002 -0.00104 0.00289 0.00185 3.06030

D111 -3.13874 0.00004 0.00462 -0.00131 0.00331 -3.13542

D112 -0.07200 0.00004 0.00062 0.00292 0.00354 -0.06846

D113 -3.07906 -0.00004 -0.00296 -0.00001 -0.00297 -3.08203

D114 0.06037 -0.00005 -0.00301 -0.00041 -0.00342 0.05695

D115 0.04909 -0.00006 -0.00496 -0.00004 -0.00500 0.04409

D116 -3.09467 -0.00008 -0.00501 -0.00044 -0.00545 -3.10012

D117 1.11333 0.00005 0.01009 0.00110 0.01120 1.12453

D118 -2.02685 0.00005 0.00978 0.00135 0.01113 -2.01571

D119 -2.02628 0.00006 0.01013 0.00147 0.01161 -2.01467

D120 1.11673 0.00006 0.00982 0.00172 0.01154 1.12827

D121 3.13725 0.00000 -0.00011 0.00023 0.00012 3.13737

D122 -0.01148 -0.00000 0.00043 0.00020 0.00063 -0.01085

D123 -0.00583 0.00001 0.00030 0.00000 0.00031 -0.00553

D124 3.12862 0.00000 0.00085 -0.00003 0.00082 3.12944

D125 -3.13624 0.00001 0.00043 -0.00015 0.00028 -3.13596

D126 -0.00330 -0.00000 0.00069 -0.00029 0.00040 -0.00290

D127 0.00683 0.00001 0.00002 0.00007 0.00009 0.00693

D128 3.13978 -0.00000 0.00028 -0.00006 0.00021 3.13999

D129 0.00204 -0.00002 -0.00040 -0.00012 -0.00051 0.00153

D130 3.13837 -0.00000 0.00002 0.00004 0.00006 3.13843

D131 -3.13237 -0.00001 -0.00094 -0.00009 -0.00103 -3.13340

D132 0.00396 0.00000 -0.00052 0.00007 -0.00045 0.00351

D133 0.00090 0.00001 0.00016 0.00016 0.00031 0.00121

D134 -3.14151 0.00001 0.00026 0.00005 0.00031 -3.14120

D135 -3.13540 -0.00000 -0.00027 -0.00000 -0.00027 -3.13567

D136 0.00537 -0.00000 -0.00016 -0.00011 -0.00027 0.00510

D137 0.00009 0.00000 0.00017 -0.00008 0.00009 0.00018

D138 -3.13720 -0.00000 -0.00004 -0.00007 -0.00012 -3.13732

D139 -3.14068 0.00001 0.00006 0.00003 0.00009 -3.14060

D140 0.00521 0.00000 -0.00015 0.00004 -0.00012 0.00510

D141 -0.00404 -0.00001 -0.00025 -0.00004 -0.00029 -0.00433

D142 -3.13693 -0.00000 -0.00051 0.00010 -0.00041 -3.13734

D143 3.13327 -0.00001 -0.00005 -0.00004 -0.00009 3.13318

D144 0.00037 0.00000 -0.00030 0.00009 -0.00021 0.00016

D145 -0.00090 -0.00001 -0.00016 -0.00016 -0.00031 -0.00121

D146 3.13540 0.00000 0.00027 0.00000 0.00027 3.13567

D147 3.14151 -0.00001 -0.00026 -0.00005 -0.00031 3.14120

D148 -0.00537 0.00000 0.00016 0.00011 0.00027 -0.00510

D149 -0.00009 -0.00000 -0.00017 0.00008 -0.00009 -0.00018

D150 3.13720 0.00000 0.00004 0.00007 0.00012 3.13732

D151 3.14068 -0.00001 -0.00006 -0.00003 -0.00009 3.14060

D152 -0.00521 -0.00000 0.00015 -0.00004 0.00012 -0.00510

D153 -0.00204 0.00002 0.00040 0.00012 0.00051 -0.00153

D154 3.13237 0.00001 0.00094 0.00009 0.00103 3.13340

D155 -3.13837 0.00000 -0.00002 -0.00004 -0.00006 -3.13843

D156 -0.00396 -0.00000 0.00052 -0.00007 0.00045 -0.00351

D157 -3.13725 -0.00000 0.00011 -0.00023 -0.00012 -3.13737

D158 0.00583 -0.00001 -0.00030 -0.00000 -0.00031 0.00553

D159 0.01148 0.00000 -0.00043 -0.00020 -0.00063 0.01085

D160 -3.12862 -0.00000 -0.00085 0.00003 -0.00082 -3.12944

D161 3.13624 -0.00001 -0.00043 0.00015 -0.00028 3.13596

D162 0.00330 0.00000 -0.00069 0.00029 -0.00040 0.00290

D163 -0.00683 -0.00001 -0.00002 -0.00007 -0.00009 -0.00693

D164 -3.13978 0.00000 -0.00028 0.00006 -0.00021 -3.13999

D165 0.00404 0.00001 0.00025 0.00004 0.00029 0.00433

D166 -3.13327 0.00001 0.00005 0.00004 0.00009 -3.13318

D167 3.13693 0.00000 0.00051 -0.00010 0.00041 3.13734

D168 -0.00037 -0.00000 0.00030 -0.00009 0.00021 -0.00016

D169 3.13613 -0.00001 -0.00030 0.00017 -0.00014 3.13599

D170 0.00315 0.00000 -0.00060 0.00036 -0.00024 0.00290

D171 -0.00683 -0.00001 -0.00000 -0.00007 -0.00007 -0.00691

D172 -3.13982 0.00001 -0.00030 0.00012 -0.00018 -3.14000

D173 -3.13709 -0.00001 -0.00007 -0.00026 -0.00033 -3.13742

D174 0.01152 0.00000 -0.00065 -0.00007 -0.00072 0.01080

D175 0.00588 -0.00001 -0.00038 -0.00002 -0.00040 0.00549

D176 -3.12869 0.00000 -0.00095 0.00017 -0.00079 -3.12948

D177 0.00400 0.00001 0.00030 0.00004 0.00034 0.00434

D178 -3.13328 0.00001 0.00004 0.00007 0.00010 -3.13317

D179 3.13693 0.00000 0.00060 -0.00015 0.00044 3.13738

D180 -0.00034 -0.00001 0.00033 -0.00013 0.00021 -0.00013

D181 -0.00006 -0.00000 -0.00022 0.00008 -0.00013 -0.00019

D182 3.14070 -0.00001 -0.00008 -0.00004 -0.00012 3.14058

D183 3.13720 0.00000 0.00005 0.00006 0.00010 3.13730

D184 -0.00522 -0.00000 0.00018 -0.00007 0.00011 -0.00511

D185 -0.00088 -0.00001 -0.00016 -0.00017 -0.00033 -0.00122

D186 3.13541 0.00000 0.00033 -0.00006 0.00027 3.13567

D187 3.14154 -0.00001 -0.00029 -0.00005 -0.00034 3.14120

D188 -0.00536 0.00000 0.00019 0.00007 0.00026 -0.00510

D189 -0.00210 0.00002 0.00046 0.00014 0.00061 -0.00149

D190 3.13244 0.00001 0.00104 -0.00005 0.00100 3.13343

D191 -3.13841 0.00001 -0.00002 0.00003 0.00001 -3.13840

D192 -0.00387 -0.00000 0.00056 -0.00016 0.00040 -0.00348

D193 -3.13613 0.00001 0.00030 -0.00017 0.00014 -3.13599

D194 -0.00315 -0.00000 0.00060 -0.00036 0.00024 -0.00290

D195 0.00683 0.00001 0.00000 0.00007 0.00007 0.00691

D196 3.13982 -0.00001 0.00030 -0.00012 0.00018 3.14000

D197 3.13709 0.00001 0.00007 0.00026 0.00033 3.13742

D198 -0.01152 -0.00000 0.00065 0.00007 0.00072 -0.01080

D199 -0.00588 0.00001 0.00038 0.00002 0.00040 -0.00549

D200 3.12869 -0.00000 0.00095 -0.00017 0.00079 3.12948

D201 -0.00400 -0.00001 -0.00030 -0.00004 -0.00034 -0.00434

D202 3.13328 -0.00001 -0.00004 -0.00007 -0.00010 3.13317

D203 -3.13693 -0.00000 -0.00060 0.00015 -0.00044 -3.13738

D204 0.00034 0.00001 -0.00033 0.00013 -0.00021 0.00013

D205 0.00006 0.00000 0.00022 -0.00008 0.00013 0.00019

D206 -3.14070 0.00001 0.00008 0.00004 0.00012 -3.14058

D207 -3.13720 -0.00000 -0.00005 -0.00006 -0.00010 -3.13730

D208 0.00522 0.00000 -0.00018 0.00007 -0.00011 0.00511

D209 0.00088 0.00001 0.00016 0.00017 0.00033 0.00122

D210 -3.13541 -0.00000 -0.00033 0.00006 -0.00027 -3.13567

D211 -3.14154 0.00001 0.00029 0.00005 0.00034 -3.14120

D212 0.00536 -0.00000 -0.00019 -0.00007 -0.00026 0.00510

D213 0.00210 -0.00002 -0.00046 -0.00014 -0.00061 0.00149

D214 -3.13244 -0.00001 -0.00104 0.00005 -0.00100 -3.13343

D215 3.13841 -0.00001 0.00002 -0.00003 -0.00001 3.13840

D216 0.00387 0.00000 -0.00056 0.00016 -0.00040 0.00348

Item Value Threshold Converged?

Maximum Force 0.000091 0.000450 YES

RMS Force 0.000032 0.000300 YES

Maximum Displacement 0.062720 0.001800 NO

RMS Displacement 0.017511 0.001200 NO

Predicted change in Energy=-9.349364D-06

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Aug 18 14:45:59 2019, MaxMem= 2013265920 cpu: 1.3

(Enter /home/kira/g09/l202.exe)

Stoichiometry C44H30N4(1-,2)

Framework group CS[SG(H2N2),X(C44H28N2)]

Deg. of freedom 116

Full point group CS NOp 2

RotChk: IX=3 Diff= 6.34D-05

Largest Abelian subgroup CS NOp 2

Largest concise Abelian subgroup CS NOp 2

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 4.259623 -0.130625 0.680973

2 6 0 2.898394 -0.000228 1.142126

3 7 0 2.117034 0.069812 -0.000000

4 6 0 2.898394 -0.000228 -1.142126

5 6 0 4.259623 -0.130625 -0.680973

6 6 0 2.460642 0.031549 -2.456395

7 6 0 1.095290 0.092792 -2.878755

8 7 0 0.000010 0.007794 -2.056310

9 6 0 -1.095305 0.092635 -2.878748

10 6 0 -0.688027 0.257917 -4.246997

11 6 0 0.687998 0.258007 -4.247006

12 6 0 2.460642 0.031549 2.456395

13 6 0 1.095290 0.092792 2.878755

14 6 0 0.687998 0.258007 4.247006

15 6 0 -0.688027 0.257917 4.246997

16 6 0 -1.095305 0.092635 2.878748

17 7 0 0.000010 0.007794 2.056310

18 6 0 -2.460630 0.031255 2.456381

19 6 0 -2.898388 -0.000779 1.142118

20 6 0 -4.259644 -0.130975 0.680977

21 6 0 -4.259644 -0.130975 -0.680977

22 6 0 -2.898388 -0.000779 -1.142118

23 7 0 -2.117010 0.068627 0.000000

24 6 0 -2.460630 0.031255 -2.456381

25 6 0 3.505973 -0.004641 -3.521375

26 6 0 4.426550 1.040769 -3.666390

27 6 0 5.404020 0.999841 -4.659409

28 6 0 5.476163 -0.088594 -5.526875

29 6 0 4.562909 -1.134983 -5.395025

30 6 0 3.586405 -1.090972 -4.403345

31 6 0 5.476163 -0.088594 5.526875

32 6 0 5.404020 0.999841 4.659409

33 6 0 4.426550 1.040769 3.666390

34 6 0 3.505973 -0.004641 3.521375

35 6 0 3.586405 -1.090972 4.403345

36 6 0 4.562909 -1.134983 5.395025

37 6 0 -3.505995 -0.004667 -3.521374

38 6 0 -3.586961 -1.091195 -4.403037

39 6 0 -4.563457 -1.134953 -5.394745

40 6 0 -5.476133 -0.088102 -5.526912

41 6 0 -5.403448 1.000528 -4.659737

42 6 0 -4.426004 1.041189 -3.666676

43 6 0 -3.505995 -0.004667 3.521374

44 6 0 -3.586961 -1.091195 4.403037

45 6 0 -4.563457 -1.134953 5.394745

46 6 0 -5.476133 -0.088102 5.526912

47 6 0 -5.403448 1.000528 4.659737

48 6 0 -4.426004 1.041189 3.666676

49 1 0 5.117832 -0.223966 1.327690

50 1 0 5.117832 -0.223966 -1.327690

51 1 0 -1.342041 0.372690 -5.098733

52 1 0 1.341990 0.372867 -5.098748

53 1 0 1.341990 0.372867 5.098748

54 1 0 -1.342041 0.372690 5.098733

55 1 0 -5.117841 -0.224268 1.327717

56 1 0 -5.117841 -0.224268 -1.327717

57 1 0 4.370071 1.893856 -2.998755

58 1 0 6.106187 1.821582 -4.756974

59 1 0 6.236806 -0.121755 -6.299995

60 1 0 4.613367 -1.988770 -6.063099

61 1 0 2.881365 -1.908976 -4.302683

62 1 0 6.236806 -0.121755 6.299995

63 1 0 6.106187 1.821582 4.756974

64 1 0 4.370071 1.893856 2.998755

65 1 0 2.881365 -1.908976 4.302683

66 1 0 4.613367 -1.988770 6.063099

67 1 0 -2.882341 -1.909532 -4.302130

68 1 0 -4.614356 -1.988892 -6.062590

69 1 0 -6.236756 -0.121056 -6.300060

70 1 0 -6.105168 1.822620 -4.757563

71 1 0 -4.369099 1.894402 -2.999237

72 1 0 -2.882341 -1.909532 4.302130

73 1 0 -4.614356 -1.988892 6.062590

74 1 0 -6.236756 -0.121056 6.300060

75 1 0 -6.105168 1.822620 4.757563

76 1 0 -4.369099 1.894402 2.999237

77 1 0 1.106676 0.095061 -0.000000

78 1 0 -1.106710 0.095950 0.000000

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

Rotational constants (GHZ): 0.0583507 0.0578333 0.0300232

Leave Link 202 at Sun Aug 18 14:45:59 2019, MaxMem= 2013265920 cpu: 0.0

(Enter /home/kira/g09/l301.exe)

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

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

There are 513 symmetry adapted cartesian basis functions of A' symmetry.

There are 489 symmetry adapted cartesian basis functions of A" symmetry.

There are 488 symmetry adapted basis functions of A' symmetry.

There are 466 symmetry adapted basis functions of A" symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 161 beta electrons

nuclear repulsion energy 5346.0410384626 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= 78 NActive= 78 NUniq= 41 SFac= 3.62D+00 NAtFMM= 60 NAOKFM=T 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= -0.2116595731 Hartrees.

Nuclear repulsion after empirical dispersion term = 5345.8293788895 Hartrees.

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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= 78.

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

Smoothing algorithm: York/Karplus (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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5712

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.19D-11

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 292

GePol: Fraction of low-weight points (<1% of avg) = 5.11%

GePol: Cavity surface area = 617.978 Ang\*\*2

GePol: Cavity volume = 629.357 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0019829451 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5345.8273959445 Hartrees.

Leave Link 301 at Sun Aug 18 14:45:59 2019, MaxMem= 2013265920 cpu: 1.0

(Enter /home/kira/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.

One-electron integral symmetry used in STVInt

NBasis= 954 RedAO= T EigKep= 8.99D-05 NBF= 488 466

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 488 466

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= 938 938 939 939 940 MxSgAt= 78 MxSgA2= 78.

Leave Link 302 at Sun Aug 18 14:46:01 2019, MaxMem= 2013265920 cpu: 10.1

(Enter /home/kira/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sun Aug 18 14:46:01 2019, MaxMem= 2013265920 cpu: 1.2

(Enter /home/kira/g09/l401.exe)

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

B after Tr= -0.000000 -0.000000 -0.000000

Rot= 1.000000 0.000000 0.000000 0.000012 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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The electronic state of the initial guess is 2-A'.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7585 S= 0.5043

Generating alternative initial guess.

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2000

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= -1914.58000922323

Leave Link 401 at Sun Aug 18 14:46:07 2019, MaxMem= 2013265920 cpu: 46.0

(Enter /home/kira/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3047318 IEndB= 3047318 NGot= 2013265920 MDV= 2011240249

LenX= 2011240249 LenY= 2010235243

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= 480000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 97880832.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.66D-15 for 5688.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.70D-15 for 2331 1891.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.22D-15 for 5708.

Iteration 1 A^-1\*A deviation from orthogonality is 6.34D-11 for 4861 4815.

E= -1914.49120272502

DIIS: error= 1.67D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.49120272502 IErMin= 1 ErrMin= 1.67D-03

ErrMax= 1.67D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.47D-03 BMatP= 4.47D-03

IDIUse=3 WtCom= 9.83D-01 WtEn= 1.67D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.446 Goal= None Shift= 0.000

Gap= 0.504 Goal= None Shift= 0.000

GapD= 0.446 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=4.69D-05 MaxDP=1.21D-03 OVMax= 8.28D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.69D-05 CP: 1.00D+00

E= -1914.49358374989 Delta-E= -0.002381024871 Rises=F Damp=F

DIIS: error= 2.25D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.49358374989 IErMin= 2 ErrMin= 2.25D-04

ErrMax= 2.25D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.09D-05 BMatP= 4.47D-03

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.25D-03

Coeff-Com: -0.729D-01 0.107D+01

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

Coeff: -0.727D-01 0.107D+01

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=8.50D-06 MaxDP=1.98D-04 DE=-2.38D-03 OVMax= 1.28D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 7.47D-06 CP: 1.00D+00 1.09D+00

E= -1914.49362331344 Delta-E= -0.000039563551 Rises=F Damp=F

DIIS: error= 4.08D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.49362331344 IErMin= 3 ErrMin= 4.08D-05

ErrMax= 4.08D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.61D-06 BMatP= 6.09D-05

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

Coeff-Com: -0.211D-01 0.237D+00 0.785D+00

Coeff: -0.211D-01 0.237D+00 0.785D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=2.25D-06 MaxDP=7.34D-05 DE=-3.96D-05 OVMax= 4.01D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.93D-06 CP: 1.00D+00 1.10D+00 8.90D-01

E= -1914.49362453012 Delta-E= -0.000001216677 Rises=F Damp=F

DIIS: error= 2.07D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.49362453012 IErMin= 4 ErrMin= 2.07D-05

ErrMax= 2.07D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.61D-06 BMatP= 5.61D-06

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

Coeff-Com: -0.541D-02 0.437D-01 0.349D+00 0.613D+00

Coeff: -0.541D-02 0.437D-01 0.349D+00 0.613D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=9.44D-07 MaxDP=4.75D-05 DE=-1.22D-06 OVMax= 2.40D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 7.65D-07 CP: 1.00D+00 1.11D+00 9.23D-01 7.51D-01

E= -1914.49362488681 Delta-E= -0.000000356697 Rises=F Damp=F

DIIS: error= 9.14D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.49362488681 IErMin= 5 ErrMin= 9.14D-06

ErrMax= 9.14D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.14D-07 BMatP= 1.61D-06

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

Coeff-Com: 0.892D-03-0.210D-01 0.400D-01 0.330D+00 0.650D+00

Coeff: 0.892D-03-0.210D-01 0.400D-01 0.330D+00 0.650D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=4.09D-07 MaxDP=1.97D-05 DE=-3.57D-07 OVMax= 8.29D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.80D-07 CP: 1.00D+00 1.11D+00 9.42D-01 8.31D-01 6.06D-01

E= -1914.49362496225 Delta-E= -0.000000075436 Rises=F Damp=F

DIIS: error= 3.17D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.49362496225 IErMin= 6 ErrMin= 3.17D-06

ErrMax= 3.17D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.16D-08 BMatP= 3.14D-07

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

Coeff-Com: 0.742D-03-0.144D-01 0.102D-01 0.176D+00 0.395D+00 0.432D+00

Coeff: 0.742D-03-0.144D-01 0.102D-01 0.176D+00 0.395D+00 0.432D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=1.14D-07 MaxDP=6.02D-06 DE=-7.54D-08 OVMax= 2.52D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 6.03D-08 CP: 1.00D+00 1.11D+00 9.43D-01 8.27D-01 6.63D-01

CP: 5.30D-01

E= -1914.49362497027 Delta-E= -0.000000008021 Rises=F Damp=F

DIIS: error= 6.35D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.49362497027 IErMin= 7 ErrMin= 6.35D-07

ErrMax= 6.35D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.99D-10 BMatP= 3.16D-08

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

Coeff-Com: 0.223D-03-0.392D-02 0.240D-04 0.428D-01 0.103D+00 0.175D+00

Coeff-Com: 0.683D+00

Coeff: 0.223D-03-0.392D-02 0.240D-04 0.428D-01 0.103D+00 0.175D+00

Coeff: 0.683D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=3.25D-08 MaxDP=1.94D-06 DE=-8.02D-09 OVMax= 7.42D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.80D-08 CP: 1.00D+00 1.11D+00 9.44D-01 8.31D-01 6.55D-01

CP: 5.93D-01 9.20D-01

E= -1914.49362497055 Delta-E= -0.000000000281 Rises=F Damp=F

DIIS: error= 3.94D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.49362497055 IErMin= 8 ErrMin= 3.94D-07

ErrMax= 3.94D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.55D-10 BMatP= 9.99D-10

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

Coeff-Com: -0.558D-04 0.136D-02-0.283D-02-0.195D-01-0.390D-01-0.310D-02

Coeff-Com: 0.434D+00 0.630D+00

Coeff: -0.558D-04 0.136D-02-0.283D-02-0.195D-01-0.390D-01-0.310D-02

Coeff: 0.434D+00 0.630D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=1.79D-08 MaxDP=8.65D-07 DE=-2.81D-10 OVMax= 4.04D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.08D-08 CP: 1.00D+00 1.11D+00 9.44D-01 8.30D-01 6.60D-01

CP: 6.07D-01 1.11D+00 7.46D-01

E= -1914.49362497080 Delta-E= -0.000000000252 Rises=F Damp=F

DIIS: error= 2.65D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.49362497080 IErMin= 9 ErrMin= 2.65D-07

ErrMax= 2.65D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.38D-11 BMatP= 4.55D-10

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

Coeff-Com: -0.442D-04 0.890D-03-0.822D-03-0.111D-01-0.248D-01-0.228D-01

Coeff-Com: 0.480D-01 0.196D+00 0.815D+00

Coeff: -0.442D-04 0.890D-03-0.822D-03-0.111D-01-0.248D-01-0.228D-01

Coeff: 0.480D-01 0.196D+00 0.815D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=8.65D-09 MaxDP=4.70D-07 DE=-2.52D-10 OVMax= 2.85D-06

Error on total polarization charges = 0.08609

SCF Done: E(UB3LYP) = -1914.49362497 A.U. after 9 cycles

NFock= 9 Conv=0.87D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7586 S= 0.5043

<L.S>= 0.000000000000E+00

KE= 1.906564496160D+03 PE=-1.517660018782D+04 EE= 6.009714670748D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.24

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7586, after 0.7500

Leave Link 502 at Sun Aug 18 14:51:01 2019, MaxMem= 2013265920 cpu: 2340.0

(Enter /home/kira/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 = 181

Leave Link 701 at Sun Aug 18 14:51:17 2019, MaxMem= 2013265920 cpu: 124.3

(Enter /home/kira/g09/l702.exe)

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

Leave Link 702 at Sun Aug 18 14:51:17 2019, MaxMem= 2013265920 cpu: 0.1

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 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= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

Petite list used in FoFCou.

Leave Link 703 at Sun Aug 18 14:52:22 2019, MaxMem= 2013265920 cpu: 520.8

(Enter /home/kira/g09/l716.exe)

Dipole =-2.68792626D-04-1.20676677D-01 7.92255150D-13

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000040781 0.000071533 -0.000056648

2 6 -0.000068113 -0.000010568 0.000125143

3 7 -0.000053747 -0.000229735 -0.000000000

4 6 -0.000068113 -0.000010568 -0.000125143

5 6 0.000040781 0.000071533 0.000056648

6 6 -0.000005645 0.000009205 0.000067799

7 6 0.000033200 -0.000060684 0.000011191

8 7 -0.000001748 0.000098991 0.000074504

9 6 -0.000024551 -0.000058567 0.000009510

10 6 0.000019315 0.000015397 -0.000004591

11 6 -0.000025826 0.000018818 -0.000003250

12 6 -0.000005645 0.000009205 -0.000067799

13 6 0.000033200 -0.000060684 -0.000011191

14 6 -0.000025826 0.000018818 0.000003250

15 6 0.000019315 0.000015397 0.000004591

16 6 -0.000024551 -0.000058567 -0.000009510

17 7 -0.000001748 0.000098991 -0.000074504

18 6 -0.000003512 0.000014792 -0.000067938

19 6 0.000068669 -0.000025898 0.000131860

20 6 -0.000039679 0.000065518 -0.000059545

21 6 -0.000039679 0.000065518 0.000059545

22 6 0.000068669 -0.000025898 -0.000131860

23 7 0.000060978 -0.000165570 0.000000000

24 6 -0.000003512 0.000014792 0.000067938

25 6 -0.000031644 -0.000053866 0.000003717

26 6 0.000022746 0.000002567 -0.000025071

27 6 0.000000866 0.000011572 0.000028658

28 6 -0.000001324 -0.000009713 -0.000012462

29 6 -0.000003692 0.000006070 -0.000003382

30 6 0.000032336 0.000032644 0.000003236

31 6 -0.000001324 -0.000009713 0.000012462

32 6 0.000000866 0.000011572 -0.000028658

33 6 0.000022746 0.000002567 0.000025071

34 6 -0.000031644 -0.000053866 -0.000003717

35 6 0.000032336 0.000032644 -0.000003236

36 6 -0.000003692 0.000006070 0.000003382

37 6 0.000039792 -0.000055311 0.000011115

38 6 -0.000032555 0.000033446 -0.000000866

39 6 0.000005450 0.000006355 -0.000001987

40 6 0.000000499 -0.000009559 -0.000013279

41 6 0.000000176 0.000011641 0.000030509

42 6 -0.000024814 0.000002848 -0.000024627

43 6 0.000039792 -0.000055311 -0.000011115

44 6 -0.000032555 0.000033446 0.000000866

45 6 0.000005450 0.000006355 0.000001987

46 6 0.000000499 -0.000009559 0.000013279

47 6 0.000000176 0.000011641 -0.000030509

48 6 -0.000024814 0.000002848 0.000024627

49 1 0.000008294 -0.000021942 0.000002197

50 1 0.000008294 -0.000021942 -0.000002197

51 1 0.000005457 0.000005544 -0.000021604

52 1 -0.000007855 0.000006011 -0.000019394

53 1 -0.000007855 0.000006011 0.000019394

54 1 0.000005457 0.000005544 0.000021604

55 1 -0.000009764 -0.000019732 0.000003183

56 1 -0.000009764 -0.000019732 -0.000003183

57 1 0.000000210 0.000001820 0.000004320

58 1 0.000005626 -0.000002153 0.000001180

59 1 0.000000318 -0.000000092 -0.000001680

60 1 -0.000002587 0.000001367 -0.000005189

61 1 -0.000005619 -0.000004583 0.000001434

62 1 0.000000318 -0.000000092 0.000001680

63 1 0.000005626 -0.000002153 -0.000001180

64 1 0.000000210 0.000001820 -0.000004320

65 1 -0.000005619 -0.000004583 -0.000001434

66 1 -0.000002587 0.000001367 0.000005189

67 1 0.000006002 -0.000004709 0.000000916

68 1 0.000003200 0.000001620 -0.000005588

69 1 -0.000000351 -0.000000176 -0.000001562

70 1 -0.000006098 -0.000002541 0.000002215

71 1 -0.000000926 0.000002234 0.000004503

72 1 0.000006002 -0.000004709 -0.000000916

73 1 0.000003200 0.000001620 0.000005588

74 1 -0.000000351 -0.000000176 0.000001562

75 1 -0.000006098 -0.000002541 -0.000002215

76 1 -0.000000926 0.000002234 -0.000004503

77 1 0.000010515 0.000132591 0.000000000

78 1 -0.000011013 0.000102921 -0.000000000

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

Cartesian Forces: Max 0.000229735 RMS 0.000038810

Leave Link 716 at Sun Aug 18 14:52:22 2019, MaxMem= 2013265920 cpu: 0.2

(Enter /home/kira/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 0.000102945 RMS 0.000019434

Search for a local minimum.

Step number 8 out of a maximum of 452

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

RMS Force = .19434D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 3 4 5 6 7

8

DE= -1.04D-05 DEPred=-9.35D-06 R= 1.11D+00

TightC=F SS= 1.41D+00 RLast= 6.04D-02 DXNew= 1.6128D+00 1.8110D-01

Trust test= 1.11D+00 RLast= 6.04D-02 DXMaxT set to 9.59D-01

ITU= 1 1 0 1 1 1 1 0

Eigenvalues --- 0.00605 0.00983 0.00988 0.00989 0.01369

Eigenvalues --- 0.01532 0.01616 0.01622 0.01625 0.01635

Eigenvalues --- 0.01659 0.01723 0.01723 0.01723 0.01729

Eigenvalues --- 0.01737 0.01751 0.01773 0.01777 0.01792

Eigenvalues --- 0.01837 0.01847 0.01852 0.01856 0.01891

Eigenvalues --- 0.01901 0.01929 0.01943 0.01949 0.01984

Eigenvalues --- 0.02011 0.02020 0.02027 0.02027 0.02068

Eigenvalues --- 0.02069 0.02070 0.02071 0.02075 0.02092

Eigenvalues --- 0.02104 0.02117 0.02118 0.02119 0.02126

Eigenvalues --- 0.02130 0.02130 0.02132 0.02132 0.02132

Eigenvalues --- 0.02138 0.02160 0.02160 0.02160 0.02160

Eigenvalues --- 0.02162 0.02162 0.02162 0.02165 0.02173

Eigenvalues --- 0.02173 0.02173 0.02178 0.02181 0.02181

Eigenvalues --- 0.02181 0.02185 0.02186 0.02187 0.02187

Eigenvalues --- 0.02210 0.02216 0.02217 0.02345 0.03360

Eigenvalues --- 0.15876 0.15929 0.15935 0.15993 0.15997

Eigenvalues --- 0.15997 0.15997 0.15997 0.15998 0.15999

Eigenvalues --- 0.15999 0.15999 0.15999 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16003 0.16025 0.16047

Eigenvalues --- 0.21820 0.22000 0.22000 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22002 0.22109 0.22759

Eigenvalues --- 0.22774 0.22816 0.22836 0.23472 0.23472

Eigenvalues --- 0.23475 0.23542 0.23829 0.24376 0.24734

Eigenvalues --- 0.24848 0.24890 0.24895 0.24973 0.24996

Eigenvalues --- 0.24997 0.24999 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25001 0.25074

Eigenvalues --- 0.26123 0.27414 0.34159 0.34185 0.34206

Eigenvalues --- 0.34633 0.35411 0.35413 0.35413 0.35413

Eigenvalues --- 0.35415 0.35415 0.35416 0.35416 0.35416

Eigenvalues --- 0.35416 0.35416 0.35422 0.35506 0.35507

Eigenvalues --- 0.35508 0.35523 0.35542 0.35545 0.35547

Eigenvalues --- 0.35715 0.36056 0.36057 0.36058 0.36115

Eigenvalues --- 0.36250 0.36251 0.36251 0.36277 0.37118

Eigenvalues --- 0.37159 0.37263 0.37294 0.37879 0.39131

Eigenvalues --- 0.39745 0.39964 0.40261 0.40420 0.40464

Eigenvalues --- 0.40771 0.41781 0.41782 0.41797 0.42065

Eigenvalues --- 0.42091 0.42093 0.42095 0.42113 0.42843

Eigenvalues --- 0.43270 0.44661 0.45272 0.45569 0.45571

Eigenvalues --- 0.45586 0.45586 0.45704 0.45768 0.45847

Eigenvalues --- 0.45866 0.45931 0.45940 0.45942 0.45948

Eigenvalues --- 0.45970 0.46651 0.46660 0.46661 0.46661

Eigenvalues --- 0.47073 0.47079 0.47086 0.47512 0.48054

Eigenvalues --- 0.48191 0.48278 0.49335 0.49434 0.49975

Eigenvalues --- 0.50727 0.50810 0.54770

En-DIIS/RFO-DIIS IScMMF= 0 using points: 8 7 6 5 4

RFO step: Lambda=-5.91754644D-07.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 2.14D-04 SmlDif= 1.00D-05

RMS Error= 0.8761743719D-04 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 0.85729 0.23436 -0.03929 -0.08510 0.03275

Iteration 1 RMS(Cart)= 0.00324723 RMS(Int)= 0.00000275

Iteration 2 RMS(Cart)= 0.00000525 RMS(Int)= 0.00000069

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000069

ITry= 1 IFail=0 DXMaxC= 1.18D-02 DCOld= 1.00D+10 DXMaxT= 9.59D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 3.17D-09 for atom 50.

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

(Linear) (Quad) (Total)

R1 2.72711 0.00005 -0.00003 0.00008 0.00005 2.72716

R2 2.57370 -0.00004 -0.00001 0.00002 0.00001 2.57371

R3 2.03835 0.00001 -0.00001 0.00002 0.00000 2.03835

R4 2.61840 0.00003 0.00002 -0.00002 -0.00001 2.61839

R5 2.61844 -0.00009 -0.00001 -0.00003 -0.00004 2.61840

R6 2.61840 0.00003 0.00002 -0.00002 -0.00001 2.61839

R7 1.90990 -0.00001 0.00002 -0.00007 -0.00005 1.90984

R8 2.72711 0.00005 -0.00003 0.00008 0.00005 2.72716

R9 2.61844 -0.00009 -0.00001 -0.00003 -0.00004 2.61840

R10 2.03835 0.00001 -0.00001 0.00002 0.00000 2.03835

R11 2.70325 -0.00003 0.00002 -0.00008 -0.00005 2.70319

R12 2.82083 0.00002 -0.00003 0.00006 0.00002 2.82085

R13 2.59332 0.00002 0.00003 0.00008 0.00011 2.59343

R14 2.71575 0.00003 0.00001 -0.00000 0.00000 2.71575

R15 2.59334 0.00002 0.00003 0.00007 0.00010 2.59345

R16 2.71575 0.00002 0.00000 -0.00000 0.00000 2.71576

R17 2.70322 -0.00004 0.00003 -0.00006 -0.00004 2.70318

R18 2.60031 -0.00003 -0.00004 0.00002 -0.00001 2.60030

R19 2.04087 0.00001 -0.00001 0.00003 0.00002 2.04089

R20 2.04087 0.00001 -0.00001 0.00003 0.00002 2.04089

R21 2.70325 -0.00003 0.00002 -0.00008 -0.00005 2.70319

R22 2.82083 0.00002 -0.00003 0.00006 0.00002 2.82085

R23 2.71575 0.00003 0.00001 -0.00000 0.00000 2.71575

R24 2.59332 0.00002 0.00003 0.00008 0.00011 2.59343

R25 2.60031 -0.00003 -0.00004 0.00002 -0.00001 2.60030

R26 2.04087 0.00001 -0.00001 0.00003 0.00002 2.04089

R27 2.71575 0.00002 0.00000 -0.00000 0.00000 2.71576

R28 2.04087 0.00001 -0.00001 0.00003 0.00002 2.04089

R29 2.59334 0.00002 0.00003 0.00007 0.00010 2.59345

R30 2.70322 -0.00004 0.00003 -0.00006 -0.00004 2.70318

R31 2.61844 -0.00010 -0.00001 -0.00002 -0.00003 2.61841

R32 2.82088 0.00001 -0.00003 0.00004 0.00001 2.82089

R33 2.72712 0.00005 -0.00003 0.00008 0.00005 2.72717

R34 2.61835 0.00003 0.00002 0.00000 0.00002 2.61837

R35 2.57372 -0.00004 -0.00001 -0.00001 -0.00002 2.57370

R36 2.03835 0.00001 -0.00001 0.00001 0.00000 2.03835

R37 2.72712 0.00005 -0.00003 0.00008 0.00005 2.72717

R38 2.03835 0.00001 -0.00001 0.00001 0.00000 2.03835

R39 2.61835 0.00003 0.00002 0.00000 0.00002 2.61837

R40 2.61844 -0.00010 -0.00001 -0.00002 -0.00003 2.61841

R41 1.90989 -0.00001 0.00002 -0.00007 -0.00005 1.90984

R42 2.82088 0.00001 -0.00003 0.00004 0.00001 2.82089

R43 2.64654 0.00003 0.00006 0.00000 0.00007 2.64661

R44 2.64862 -0.00002 0.00005 -0.00010 -0.00006 2.64857

R45 2.63426 -0.00001 -0.00002 -0.00002 -0.00004 2.63422

R46 2.04988 0.00000 -0.00001 0.00002 0.00001 2.04989

R47 2.63371 0.00001 -0.00000 0.00003 0.00003 2.63374

R48 2.05087 0.00000 0.00000 -0.00000 0.00000 2.05087

R49 2.63639 -0.00000 0.00000 -0.00002 -0.00002 2.63637

R50 2.05050 0.00000 0.00000 0.00000 0.00000 2.05050

R51 2.63136 0.00000 -0.00003 0.00003 -0.00000 2.63135

R52 2.05087 0.00000 0.00000 0.00000 0.00000 2.05088

R53 2.04959 0.00001 -0.00001 0.00003 0.00002 2.04961

R54 2.63371 0.00001 -0.00000 0.00003 0.00003 2.63374

R55 2.63639 -0.00000 0.00000 -0.00002 -0.00002 2.63637

R56 2.05050 0.00000 0.00000 0.00000 0.00000 2.05050

R57 2.63426 -0.00001 -0.00002 -0.00002 -0.00004 2.63422

R58 2.05087 0.00000 0.00000 -0.00000 0.00000 2.05087

R59 2.64654 0.00003 0.00006 0.00000 0.00007 2.64661

R60 2.04988 0.00000 -0.00001 0.00002 0.00001 2.04989

R61 2.64862 -0.00002 0.00005 -0.00010 -0.00006 2.64857

R62 2.63136 0.00000 -0.00003 0.00003 -0.00000 2.63135

R63 2.04959 0.00001 -0.00001 0.00003 0.00002 2.04961

R64 2.05087 0.00000 0.00000 0.00000 0.00000 2.05088

R65 2.64860 -0.00002 0.00005 -0.00009 -0.00004 2.64856

R66 2.64652 0.00003 0.00007 0.00001 0.00008 2.64660

R67 2.63137 0.00000 -0.00003 0.00002 -0.00001 2.63136

R68 2.04959 0.00001 -0.00001 0.00003 0.00002 2.04960

R69 2.63638 -0.00000 0.00000 -0.00002 -0.00002 2.63637

R70 2.05087 0.00000 0.00000 0.00000 0.00000 2.05088

R71 2.63371 0.00001 -0.00001 0.00004 0.00003 2.63374

R72 2.05050 0.00000 0.00000 0.00000 0.00001 2.05050

R73 2.63427 -0.00001 -0.00002 -0.00003 -0.00005 2.63422

R74 2.05087 0.00000 0.00000 -0.00000 0.00000 2.05087

R75 2.04988 0.00000 -0.00001 0.00002 0.00001 2.04989

R76 2.64860 -0.00002 0.00005 -0.00009 -0.00004 2.64856

R77 2.64652 0.00003 0.00007 0.00001 0.00008 2.64660

R78 2.63137 0.00000 -0.00003 0.00002 -0.00001 2.63136

R79 2.04959 0.00001 -0.00001 0.00003 0.00002 2.04960

R80 2.63638 -0.00000 0.00000 -0.00002 -0.00002 2.63637

R81 2.05087 0.00000 0.00000 0.00000 0.00000 2.05088

R82 2.63371 0.00001 -0.00001 0.00004 0.00003 2.63374

R83 2.05050 0.00000 0.00000 0.00000 0.00001 2.05050

R84 2.63427 -0.00001 -0.00002 -0.00003 -0.00005 2.63422

R85 2.05087 0.00000 0.00000 -0.00000 0.00000 2.05087

R86 2.04988 0.00000 -0.00001 0.00002 0.00001 2.04989

A1 1.89605 0.00001 -0.00001 0.00003 0.00002 1.89607

A2 2.17330 0.00000 0.00005 -0.00002 0.00004 2.17334

A3 2.21375 -0.00001 -0.00004 -0.00002 -0.00006 2.21369

A4 1.84739 -0.00000 0.00006 -0.00014 -0.00008 1.84731

A5 2.21826 -0.00001 -0.00003 0.00007 0.00004 2.21830

A6 2.21746 0.00001 -0.00002 0.00007 0.00004 2.21750

A7 1.93787 -0.00001 -0.00009 0.00019 0.00010 1.93798

A8 2.17123 0.00001 0.00006 0.00007 0.00013 2.17136

A9 2.17123 0.00001 0.00006 0.00007 0.00013 2.17136

A10 1.84739 -0.00000 0.00006 -0.00014 -0.00008 1.84731

A11 2.21746 0.00001 -0.00002 0.00007 0.00004 2.21750

A12 2.21826 -0.00001 -0.00003 0.00007 0.00004 2.21830

A13 1.89605 0.00001 -0.00001 0.00003 0.00002 1.89607

A14 2.21375 -0.00001 -0.00004 -0.00002 -0.00006 2.21369

A15 2.17330 0.00000 0.00005 -0.00002 0.00004 2.17334

A16 2.19268 -0.00002 -0.00013 0.00006 -0.00008 2.19261

A17 2.04308 -0.00002 0.00000 -0.00007 -0.00007 2.04301

A18 2.04742 0.00004 0.00013 0.00002 0.00015 2.04757

A19 2.19219 -0.00002 -0.00006 -0.00001 -0.00008 2.19211

A20 2.16100 0.00001 0.00004 0.00009 0.00014 2.16114

A21 1.92999 0.00001 0.00002 -0.00008 -0.00006 1.92993

A22 1.84836 -0.00003 -0.00006 0.00005 -0.00000 1.84836

A23 1.92997 0.00002 0.00002 -0.00006 -0.00004 1.92992

A24 2.19221 -0.00002 -0.00006 -0.00005 -0.00010 2.19210

A25 2.16101 0.00000 0.00004 0.00010 0.00015 2.16116

A26 1.85815 -0.00000 0.00001 0.00002 0.00002 1.85817

A27 2.20367 0.00002 0.00003 0.00010 0.00013 2.20381

A28 2.22127 -0.00002 -0.00004 -0.00012 -0.00015 2.22112

A29 1.85813 0.00000 -0.00001 0.00005 0.00004 1.85817

A30 2.20369 0.00002 0.00004 0.00008 0.00012 2.20380

A31 2.22128 -0.00002 -0.00004 -0.00012 -0.00016 2.22112

A32 2.19268 -0.00002 -0.00013 0.00006 -0.00008 2.19261

A33 2.04308 -0.00002 0.00000 -0.00007 -0.00007 2.04301

A34 2.04742 0.00004 0.00013 0.00002 0.00015 2.04757

A35 2.16100 0.00001 0.00004 0.00009 0.00014 2.16114

A36 2.19219 -0.00002 -0.00006 -0.00001 -0.00008 2.19211

A37 1.92999 0.00001 0.00002 -0.00008 -0.00006 1.92993

A38 1.85813 0.00000 -0.00001 0.00005 0.00004 1.85817

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A40 2.22128 -0.00002 -0.00004 -0.00012 -0.00016 2.22112

A41 1.85815 -0.00000 0.00001 0.00002 0.00002 1.85817

A42 2.22127 -0.00002 -0.00004 -0.00012 -0.00015 2.22112

A43 2.20367 0.00002 0.00003 0.00010 0.00013 2.20381

A44 1.92997 0.00002 0.00002 -0.00006 -0.00004 1.92992

A45 2.16101 0.00000 0.00004 0.00010 0.00015 2.16116

A46 2.19221 -0.00002 -0.00006 -0.00005 -0.00010 2.19210

A47 1.84836 -0.00003 -0.00006 0.00005 -0.00000 1.84836

A48 2.19271 -0.00002 -0.00013 0.00004 -0.00009 2.19261

A49 2.04742 0.00004 0.00014 0.00002 0.00016 2.04758

A50 2.04306 -0.00002 -0.00001 -0.00006 -0.00007 2.04299

A51 2.21828 -0.00001 -0.00003 0.00006 0.00003 2.21831

A52 2.21745 0.00001 -0.00002 0.00008 0.00005 2.21751

A53 1.84738 0.00000 0.00006 -0.00013 -0.00007 1.84731

A54 1.89604 0.00001 -0.00001 0.00004 0.00003 1.89607

A55 2.17329 0.00000 0.00004 0.00000 0.00004 2.17333

A56 2.21378 -0.00001 -0.00003 -0.00005 -0.00007 2.21370

A57 1.89604 0.00001 -0.00001 0.00004 0.00003 1.89607

A58 2.21378 -0.00001 -0.00003 -0.00005 -0.00007 2.21370

A59 2.17329 0.00000 0.00004 0.00000 0.00004 2.17333

A60 1.84738 0.00000 0.00006 -0.00013 -0.00007 1.84731

A61 2.21828 -0.00001 -0.00003 0.00006 0.00003 2.21831

A62 2.21745 0.00001 -0.00002 0.00008 0.00005 2.21751

A63 1.93791 -0.00002 -0.00009 0.00017 0.00008 1.93799

A64 2.17134 0.00001 0.00006 0.00004 0.00010 2.17143

A65 2.17134 0.00001 0.00006 0.00004 0.00010 2.17143

A66 2.19271 -0.00002 -0.00013 0.00004 -0.00009 2.19261

A67 2.04742 0.00004 0.00014 0.00002 0.00016 2.04758

A68 2.04306 -0.00002 -0.00001 -0.00006 -0.00007 2.04299

A69 2.11308 -0.00002 0.00004 -0.00020 -0.00017 2.11292

A70 2.10357 0.00005 0.00005 0.00017 0.00022 2.10379

A71 2.06653 -0.00002 -0.00008 0.00003 -0.00005 2.06648

A72 2.10920 0.00002 0.00005 0.00000 0.00005 2.10925

A73 2.08184 -0.00001 -0.00001 -0.00003 -0.00004 2.08180

A74 2.09213 -0.00001 -0.00003 0.00002 -0.00001 2.09212

A75 2.09741 -0.00001 -0.00000 -0.00003 -0.00003 2.09738

A76 2.08919 0.00001 0.00000 0.00003 0.00004 2.08923

A77 2.09657 -0.00000 -0.00000 -0.00000 -0.00001 2.09657

A78 2.08638 -0.00001 -0.00001 0.00000 -0.00001 2.08638

A79 2.09859 0.00000 0.00000 0.00001 0.00001 2.09860

A80 2.09821 0.00000 0.00001 -0.00001 -0.00000 2.09821

A81 2.09748 0.00000 0.00001 0.00000 0.00001 2.09749

A82 2.09606 -0.00000 -0.00001 -0.00001 -0.00002 2.09605

A83 2.08964 -0.00000 -0.00000 0.00001 0.00000 2.08964

A84 2.10935 0.00001 0.00004 -0.00001 0.00003 2.10937

A85 2.08157 -0.00001 -0.00002 -0.00002 -0.00003 2.08154

A86 2.09224 -0.00000 -0.00002 0.00003 0.00001 2.09224

A87 2.08638 -0.00001 -0.00001 0.00000 -0.00001 2.08638

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A90 2.09741 -0.00001 -0.00000 -0.00003 -0.00003 2.09738

A91 2.09657 -0.00000 -0.00000 -0.00000 -0.00001 2.09657

A92 2.08919 0.00001 0.00000 0.00003 0.00004 2.08923

A93 2.10920 0.00002 0.00005 0.00000 0.00005 2.10925

A94 2.09213 -0.00001 -0.00003 0.00002 -0.00001 2.09212

A95 2.08184 -0.00001 -0.00001 -0.00003 -0.00004 2.08180

A96 2.11308 -0.00002 0.00004 -0.00020 -0.00017 2.11292

A97 2.10357 0.00005 0.00005 0.00017 0.00022 2.10379

A98 2.06653 -0.00002 -0.00008 0.00003 -0.00005 2.06648

A99 2.10935 0.00001 0.00004 -0.00001 0.00003 2.10937

A100 2.08157 -0.00001 -0.00002 -0.00002 -0.00003 2.08154

A101 2.09224 -0.00000 -0.00002 0.00003 0.00001 2.09224

A102 2.09748 0.00000 0.00001 0.00000 0.00001 2.09749

A103 2.09606 -0.00000 -0.00001 -0.00001 -0.00002 2.09605

A104 2.08964 -0.00000 -0.00000 0.00001 0.00000 2.08964

A105 2.10354 0.00005 0.00005 0.00020 0.00025 2.10379

A106 2.11308 -0.00003 0.00003 -0.00021 -0.00018 2.11290

A107 2.06656 -0.00002 -0.00008 0.00001 -0.00007 2.06649

A108 2.10933 0.00001 0.00004 -0.00000 0.00003 2.10937

A109 2.08157 -0.00001 -0.00002 -0.00001 -0.00003 2.08154

A110 2.09225 -0.00000 -0.00002 0.00002 -0.00000 2.09225

A111 2.09747 0.00000 0.00001 0.00001 0.00002 2.09749

A112 2.08965 -0.00000 -0.00000 0.00000 0.00000 2.08965

A113 2.09606 -0.00000 -0.00001 -0.00001 -0.00002 2.09604

A114 2.08640 -0.00001 -0.00001 -0.00000 -0.00001 2.08638

A115 2.09820 0.00000 0.00001 -0.00001 -0.00000 2.09820

A116 2.09859 0.00000 0.00000 0.00001 0.00001 2.09860

A117 2.09741 -0.00000 -0.00000 -0.00002 -0.00003 2.09738

A118 2.09657 0.00000 -0.00000 0.00000 -0.00000 2.09656

A119 2.08920 0.00000 0.00001 0.00003 0.00003 2.08923

A120 2.10918 0.00002 0.00005 0.00001 0.00006 2.10924

A121 2.08184 -0.00001 -0.00001 -0.00002 -0.00004 2.08180

A122 2.09215 -0.00001 -0.00003 0.00001 -0.00002 2.09212

A123 2.10354 0.00005 0.00005 0.00020 0.00025 2.10379

A124 2.11308 -0.00003 0.00003 -0.00021 -0.00018 2.11290

A125 2.06656 -0.00002 -0.00008 0.00001 -0.00007 2.06649

A126 2.10933 0.00001 0.00004 -0.00000 0.00003 2.10937

A127 2.08157 -0.00001 -0.00002 -0.00001 -0.00003 2.08154

A128 2.09225 -0.00000 -0.00002 0.00002 -0.00000 2.09225

A129 2.09747 0.00000 0.00001 0.00001 0.00002 2.09749

A130 2.08965 -0.00000 -0.00000 0.00000 0.00000 2.08965

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A132 2.08640 -0.00001 -0.00001 -0.00000 -0.00001 2.08638

A133 2.09820 0.00000 0.00001 -0.00001 -0.00000 2.09820

A134 2.09859 0.00000 0.00000 0.00001 0.00001 2.09860

A135 2.09741 -0.00000 -0.00000 -0.00002 -0.00003 2.09738

A136 2.09657 0.00000 -0.00000 0.00000 -0.00000 2.09656

A137 2.08920 0.00000 0.00001 0.00003 0.00003 2.08923

A138 2.10918 0.00002 0.00005 0.00001 0.00006 2.10924

A139 2.08184 -0.00001 -0.00001 -0.00002 -0.00004 2.08180

A140 2.09215 -0.00001 -0.00003 0.00001 -0.00002 2.09212

D1 0.00359 0.00001 0.00023 0.00051 0.00074 0.00434

D2 3.13244 0.00003 0.00058 0.00099 0.00157 3.13402

D3 -3.12553 0.00001 0.00027 0.00083 0.00110 -3.12443

D4 0.00332 0.00003 0.00062 0.00131 0.00193 0.00525

D5 0.00000 0.00000 -0.00000 0.00000 -0.00000 0.00000

D6 -3.12876 -0.00000 0.00004 0.00032 0.00037 -3.12839

D7 3.12876 0.00000 -0.00004 -0.00032 -0.00037 3.12839

D8 -0.00000 -0.00000 -0.00000 -0.00000 0.00000 0.00000

D9 -0.00601 -0.00001 -0.00038 -0.00086 -0.00125 -0.00726

D10 3.05749 0.00006 -0.00002 0.00382 0.00380 3.06129

D11 -3.13487 -0.00003 -0.00074 -0.00134 -0.00207 -3.13694

D12 -0.07137 0.00004 -0.00037 0.00335 0.00298 -0.06840

D13 -3.08173 -0.00002 0.00051 -0.00134 -0.00083 -3.08256

D14 0.05716 -0.00001 0.00057 -0.00106 -0.00049 0.05667

D15 0.04450 0.00000 0.00094 -0.00076 0.00017 0.04468

D16 -3.09979 0.00001 0.00100 -0.00049 0.00051 -3.09928

D17 0.00601 0.00001 0.00038 0.00086 0.00125 0.00726

D18 3.13487 0.00003 0.00074 0.00134 0.00207 3.13694

D19 -3.05749 -0.00006 0.00002 -0.00382 -0.00380 -3.06129

D20 0.07137 -0.00004 0.00037 -0.00335 -0.00298 0.06840

D21 -0.00359 -0.00001 -0.00023 -0.00051 -0.00074 -0.00434

D22 3.12553 -0.00001 -0.00027 -0.00083 -0.00110 3.12443

D23 -3.13244 -0.00003 -0.00058 -0.00099 -0.00157 -3.13402

D24 -0.00332 -0.00003 -0.00062 -0.00131 -0.00193 -0.00525

D25 -0.04450 -0.00000 -0.00094 0.00076 -0.00017 -0.04468

D26 3.09979 -0.00001 -0.00100 0.00049 -0.00051 3.09928

D27 3.08173 0.00002 -0.00051 0.00134 0.00083 3.08256

D28 -0.05716 0.00001 -0.00057 0.00106 0.00049 -0.05667

D29 -0.10961 0.00000 -0.00116 0.00144 0.00028 -0.10933

D30 3.02910 -0.00001 -0.00131 0.00126 -0.00005 3.02906

D31 3.02927 0.00001 -0.00110 0.00172 0.00062 3.02989

D32 -0.11520 0.00000 -0.00124 0.00154 0.00029 -0.11491

D33 -1.12758 0.00002 0.00096 0.00054 0.00150 -1.12608

D34 2.01534 0.00002 0.00102 0.00038 0.00140 2.01674

D35 2.01649 0.00002 0.00090 0.00029 0.00119 2.01768

D36 -1.12378 0.00001 0.00096 0.00013 0.00109 -1.12268

D37 -3.12643 0.00003 0.00060 0.00059 0.00119 -3.12524

D38 0.01772 0.00004 0.00073 0.00075 0.00148 0.01920

D39 3.13297 -0.00001 -0.00032 -0.00035 -0.00066 3.13230

D40 -0.02225 -0.00000 -0.00032 -0.00002 -0.00034 -0.02259

D41 -0.01113 -0.00002 -0.00044 -0.00051 -0.00095 -0.01207

D42 3.11684 -0.00001 -0.00044 -0.00018 -0.00062 3.11622

D43 -0.01773 -0.00004 -0.00074 -0.00072 -0.00146 -0.01919

D44 3.12648 -0.00003 -0.00064 -0.00062 -0.00126 3.12522

D45 0.01114 0.00002 0.00048 0.00042 0.00090 0.01204

D46 -3.11683 0.00001 0.00044 0.00016 0.00060 -3.11623

D47 -3.13301 0.00001 0.00038 0.00032 0.00070 -3.13231

D48 0.02220 0.00000 0.00034 0.00006 0.00040 0.02260

D49 0.10938 -0.00000 0.00117 -0.00138 -0.00022 0.10916

D50 -3.02960 -0.00001 0.00100 -0.00153 -0.00053 -3.03012

D51 -3.02927 0.00001 0.00128 -0.00126 0.00002 -3.02925

D52 0.11494 -0.00000 0.00112 -0.00141 -0.00029 0.11465

D53 -0.00001 0.00000 -0.00002 0.00005 0.00003 0.00002

D54 -3.12779 -0.00001 -0.00002 -0.00028 -0.00031 -3.12810

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D56 0.00000 0.00000 0.00002 -0.00002 -0.00000 0.00000

D57 -3.02910 0.00001 0.00131 -0.00126 0.00005 -3.02906

D58 0.10961 -0.00000 0.00116 -0.00144 -0.00028 0.10933

D59 0.11520 -0.00000 0.00124 -0.00154 -0.00029 0.11491

D60 -3.02927 -0.00001 0.00110 -0.00172 -0.00062 -3.02989

D61 1.12758 -0.00002 -0.00096 -0.00054 -0.00150 1.12608

D62 -2.01534 -0.00002 -0.00102 -0.00038 -0.00140 -2.01674

D63 -2.01649 -0.00002 -0.00090 -0.00029 -0.00119 -2.01768

D64 1.12378 -0.00001 -0.00096 -0.00013 -0.00109 1.12268

D65 -3.13297 0.00001 0.00032 0.00035 0.00066 -3.13230

D66 0.02225 0.00000 0.00032 0.00002 0.00034 0.02259

D67 0.01113 0.00002 0.00044 0.00051 0.00095 0.01207

D68 -3.11684 0.00001 0.00044 0.00018 0.00062 -3.11622

D69 3.12643 -0.00003 -0.00060 -0.00059 -0.00119 3.12524

D70 -0.01772 -0.00004 -0.00073 -0.00075 -0.00148 -0.01920

D71 0.00001 -0.00000 0.00002 -0.00005 -0.00003 -0.00002

D72 -3.12779 -0.00001 -0.00002 -0.00032 -0.00033 -3.12812

D73 3.12779 0.00001 0.00002 0.00028 0.00031 3.12810

D74 -0.00000 -0.00000 -0.00002 0.00002 0.00000 -0.00000

D75 -0.01114 -0.00002 -0.00048 -0.00042 -0.00090 -0.01204

D76 3.13301 -0.00001 -0.00038 -0.00032 -0.00070 3.13231

D77 3.11683 -0.00001 -0.00044 -0.00016 -0.00060 3.11623

D78 -0.02220 -0.00000 -0.00034 -0.00006 -0.00040 -0.02260

D79 0.01773 0.00004 0.00074 0.00072 0.00146 0.01919

D80 -3.12648 0.00003 0.00064 0.00062 0.00126 -3.12522

D81 3.02927 -0.00001 -0.00128 0.00126 -0.00002 3.02925

D82 -0.11494 0.00000 -0.00112 0.00141 0.00029 -0.11465

D83 -0.10938 0.00000 -0.00117 0.00138 0.00022 -0.10916

D84 3.02960 0.00001 -0.00100 0.00153 0.00053 3.03012

D85 3.08203 0.00002 -0.00053 0.00121 0.00068 3.08271

D86 -0.04409 -0.00001 -0.00090 0.00046 -0.00044 -0.04453

D87 -0.05695 0.00001 -0.00069 0.00106 0.00037 -0.05658

D88 3.10012 -0.00002 -0.00106 0.00031 -0.00075 3.09937

D89 -1.12453 0.00002 0.00130 0.00022 0.00152 -1.12301

D90 2.01571 0.00002 0.00124 0.00039 0.00163 2.01734

D91 2.01467 0.00003 0.00144 0.00036 0.00180 2.01647

D92 -1.12827 0.00003 0.00138 0.00053 0.00191 -1.12636

D93 -3.13273 -0.00003 -0.00061 -0.00091 -0.00152 -3.13425

D94 -0.00370 -0.00003 -0.00060 -0.00128 -0.00189 -0.00559

D95 -0.00398 -0.00001 -0.00030 -0.00028 -0.00058 -0.00456

D96 3.12506 -0.00000 -0.00030 -0.00066 -0.00095 3.12410

D97 3.13542 0.00003 0.00081 0.00110 0.00191 3.13733

D98 0.06846 -0.00003 0.00018 -0.00233 -0.00215 0.06631

D99 0.00666 0.00001 0.00050 0.00047 0.00098 0.00764

D100 -3.06030 -0.00005 -0.00013 -0.00295 -0.00308 -3.06338

D101 -0.00000 0.00000 0.00000 0.00000 -0.00000 -0.00000

D102 3.12866 0.00000 0.00001 -0.00039 -0.00038 3.12828

D103 -3.12866 -0.00000 -0.00001 0.00039 0.00038 -3.12828

D104 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D105 0.00398 0.00001 0.00030 0.00028 0.00058 0.00456

D106 3.13273 0.00003 0.00061 0.00091 0.00152 3.13425

D107 -3.12506 0.00000 0.00030 0.00066 0.00095 -3.12410

D108 0.00370 0.00003 0.00060 0.00128 0.00189 0.00559

D109 -0.00666 -0.00001 -0.00050 -0.00047 -0.00098 -0.00764

D110 3.06030 0.00005 0.00013 0.00295 0.00308 3.06338

D111 -3.13542 -0.00003 -0.00081 -0.00110 -0.00191 -3.13733

D112 -0.06846 0.00003 -0.00018 0.00233 0.00215 -0.06631

D113 -3.08203 -0.00002 0.00053 -0.00121 -0.00068 -3.08271

D114 0.05695 -0.00001 0.00069 -0.00106 -0.00037 0.05658

D115 0.04409 0.00001 0.00090 -0.00046 0.00044 0.04453

D116 -3.10012 0.00002 0.00106 -0.00031 0.00075 -3.09937

D117 1.12453 -0.00002 -0.00130 -0.00022 -0.00152 1.12301

D118 -2.01571 -0.00002 -0.00124 -0.00039 -0.00163 -2.01734

D119 -2.01467 -0.00003 -0.00144 -0.00036 -0.00180 -2.01647

D120 1.12827 -0.00003 -0.00138 -0.00053 -0.00191 1.12636

D121 3.13737 -0.00000 0.00005 -0.00015 -0.00011 3.13726

D122 -0.01085 0.00000 -0.00014 0.00018 0.00004 -0.01081

D123 -0.00553 -0.00000 -0.00001 0.00001 -0.00001 -0.00553

D124 3.12944 0.00000 -0.00020 0.00034 0.00014 3.12958

D125 -3.13596 -0.00000 -0.00013 0.00004 -0.00009 -3.13605

D126 -0.00290 0.00000 -0.00016 0.00020 0.00005 -0.00285

D127 0.00693 -0.00001 -0.00007 -0.00012 -0.00019 0.00674

D128 3.13999 0.00000 -0.00010 0.00004 -0.00005 3.13994

D129 0.00153 0.00001 0.00008 0.00008 0.00017 0.00169

D130 3.13843 0.00001 -0.00005 0.00022 0.00017 3.13860

D131 -3.13340 0.00000 0.00027 -0.00025 0.00001 -3.13339

D132 0.00351 -0.00000 0.00013 -0.00012 0.00002 0.00352

D133 0.00121 -0.00001 -0.00007 -0.00006 -0.00013 0.00108

D134 -3.14120 -0.00001 -0.00007 -0.00005 -0.00012 -3.14132

D135 -3.13567 -0.00000 0.00006 -0.00019 -0.00013 -3.13581

D136 0.00510 -0.00000 0.00007 -0.00019 -0.00012 0.00498

D137 0.00018 -0.00000 -0.00000 -0.00005 -0.00006 0.00012

D138 -3.13732 -0.00000 0.00004 -0.00009 -0.00005 -3.13737

D139 -3.14060 -0.00000 -0.00001 -0.00006 -0.00007 -3.14067

D140 0.00510 -0.00000 0.00004 -0.00010 -0.00006 0.00504

D141 -0.00433 0.00001 0.00008 0.00014 0.00022 -0.00411

D142 -3.13734 0.00000 0.00011 -0.00002 0.00009 -3.13725

D143 3.13318 0.00001 0.00003 0.00018 0.00021 3.13339

D144 0.00016 0.00000 0.00006 0.00002 0.00008 0.00024

D145 -0.00121 0.00001 0.00007 0.00006 0.00013 -0.00108

D146 3.13567 0.00000 -0.00006 0.00019 0.00013 3.13581

D147 3.14120 0.00001 0.00007 0.00005 0.00012 3.14132

D148 -0.00510 0.00000 -0.00007 0.00019 0.00012 -0.00498

D149 -0.00018 0.00000 0.00000 0.00005 0.00006 -0.00012

D150 3.13732 0.00000 -0.00004 0.00009 0.00005 3.13737

D151 3.14060 0.00000 0.00001 0.00006 0.00007 3.14067

D152 -0.00510 0.00000 -0.00004 0.00010 0.00006 -0.00504

D153 -0.00153 -0.00001 -0.00008 -0.00008 -0.00017 -0.00169

D154 3.13340 -0.00000 -0.00027 0.00025 -0.00001 3.13339

D155 -3.13843 -0.00001 0.00005 -0.00022 -0.00017 -3.13860

D156 -0.00351 0.00000 -0.00013 0.00012 -0.00002 -0.00352

D157 -3.13737 0.00000 -0.00005 0.00015 0.00011 -3.13726

D158 0.00553 0.00000 0.00001 -0.00001 0.00001 0.00553

D159 0.01085 -0.00000 0.00014 -0.00018 -0.00004 0.01081

D160 -3.12944 -0.00000 0.00020 -0.00034 -0.00014 -3.12958

D161 3.13596 0.00000 0.00013 -0.00004 0.00009 3.13605

D162 0.00290 -0.00000 0.00016 -0.00020 -0.00005 0.00285

D163 -0.00693 0.00001 0.00007 0.00012 0.00019 -0.00674

D164 -3.13999 -0.00000 0.00010 -0.00004 0.00005 -3.13994

D165 0.00433 -0.00001 -0.00008 -0.00014 -0.00022 0.00411

D166 -3.13318 -0.00001 -0.00003 -0.00018 -0.00021 -3.13339

D167 3.13734 -0.00000 -0.00011 0.00002 -0.00009 3.13725

D168 -0.00016 -0.00000 -0.00006 -0.00002 -0.00008 -0.00024

D169 3.13599 0.00001 0.00013 -0.00004 0.00009 3.13608

D170 0.00290 -0.00000 0.00012 -0.00015 -0.00003 0.00287

D171 -0.00691 0.00001 0.00007 0.00013 0.00020 -0.00671

D172 -3.14000 -0.00000 0.00006 0.00001 0.00008 -3.13992

D173 -3.13742 0.00000 -0.00001 0.00013 0.00013 -3.13730

D174 0.01080 -0.00000 0.00014 -0.00013 0.00000 0.01080

D175 0.00549 0.00000 0.00005 -0.00003 0.00002 0.00550

D176 -3.12948 -0.00000 0.00020 -0.00030 -0.00011 -3.12958

D177 0.00434 -0.00001 -0.00011 -0.00013 -0.00024 0.00409

D178 -3.13317 -0.00001 -0.00005 -0.00017 -0.00022 -3.13340

D179 3.13738 -0.00000 -0.00011 -0.00002 -0.00012 3.13725

D180 -0.00013 -0.00000 -0.00004 -0.00006 -0.00010 -0.00024

D181 -0.00019 0.00000 0.00003 0.00004 0.00007 -0.00012

D182 3.14058 0.00000 0.00003 0.00006 0.00009 3.14067

D183 3.13730 0.00000 -0.00003 0.00009 0.00005 3.13736

D184 -0.00511 0.00000 -0.00004 0.00010 0.00007 -0.00504

D185 -0.00122 0.00001 0.00009 0.00005 0.00014 -0.00108

D186 3.13567 0.00000 -0.00007 0.00021 0.00013 3.13581

D187 3.14120 0.00001 0.00009 0.00003 0.00012 3.14132

D188 -0.00510 0.00000 -0.00007 0.00019 0.00012 -0.00498

D189 -0.00149 -0.00001 -0.00013 -0.00005 -0.00018 -0.00168

D190 3.13343 -0.00000 -0.00028 0.00022 -0.00006 3.13337

D191 -3.13840 -0.00001 0.00003 -0.00021 -0.00018 -3.13858

D192 -0.00348 0.00000 -0.00012 0.00006 -0.00006 -0.00353

D193 -3.13599 -0.00001 -0.00013 0.00004 -0.00009 -3.13608

D194 -0.00290 0.00000 -0.00012 0.00015 0.00003 -0.00287

D195 0.00691 -0.00001 -0.00007 -0.00013 -0.00020 0.00671

D196 3.14000 0.00000 -0.00006 -0.00001 -0.00008 3.13992

D197 3.13742 -0.00000 0.00001 -0.00013 -0.00013 3.13730

D198 -0.01080 0.00000 -0.00014 0.00013 -0.00000 -0.01080

D199 -0.00549 -0.00000 -0.00005 0.00003 -0.00002 -0.00550

D200 3.12948 0.00000 -0.00020 0.00030 0.00011 3.12958

D201 -0.00434 0.00001 0.00011 0.00013 0.00024 -0.00409

D202 3.13317 0.00001 0.00005 0.00017 0.00022 3.13340

D203 -3.13738 0.00000 0.00011 0.00002 0.00012 -3.13725

D204 0.00013 0.00000 0.00004 0.00006 0.00010 0.00024

D205 0.00019 -0.00000 -0.00003 -0.00004 -0.00007 0.00012

D206 -3.14058 -0.00000 -0.00003 -0.00006 -0.00009 -3.14067

D207 -3.13730 -0.00000 0.00003 -0.00009 -0.00005 -3.13736

D208 0.00511 -0.00000 0.00004 -0.00010 -0.00007 0.00504

D209 0.00122 -0.00001 -0.00009 -0.00005 -0.00014 0.00108

D210 -3.13567 -0.00000 0.00007 -0.00021 -0.00013 -3.13581

D211 -3.14120 -0.00001 -0.00009 -0.00003 -0.00012 -3.14132

D212 0.00510 -0.00000 0.00007 -0.00019 -0.00012 0.00498

D213 0.00149 0.00001 0.00013 0.00005 0.00018 0.00168

D214 -3.13343 0.00000 0.00028 -0.00022 0.00006 -3.13337

D215 3.13840 0.00001 -0.00003 0.00021 0.00018 3.13858

D216 0.00348 -0.00000 0.00012 -0.00006 0.00006 0.00353

Item Value Threshold Converged?

Maximum Force 0.000103 0.000450 YES

RMS Force 0.000019 0.000300 YES

Maximum Displacement 0.011820 0.001800 NO

RMS Displacement 0.003247 0.001200 NO

Predicted change in Energy=-1.687475D-06

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Aug 18 14:52:22 2019, MaxMem= 2013265920 cpu: 1.4

(Enter /home/kira/g09/l202.exe)

Stoichiometry C44H30N4(1-,2)

Framework group CS[SG(H2N2),X(C44H28N2)]

Deg. of freedom 116

Full point group CS NOp 2

RotChk: IX=3 Diff= 2.38D-05

Largest Abelian subgroup CS NOp 2

Largest concise Abelian subgroup CS NOp 2

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 4.259400 -0.134252 0.680974

2 6 0 2.898207 -0.003329 1.142163

3 7 0 2.116847 0.066019 0.000000

4 6 0 2.898207 -0.003329 -1.142163

5 6 0 4.259400 -0.134252 -0.680974

6 6 0 2.460617 0.030349 -2.456418

7 6 0 1.095345 0.093019 -2.878729

8 7 0 0.000010 0.008036 -2.056258

9 6 0 -1.095337 0.092919 -2.878737

10 6 0 -0.688006 0.260160 -4.246735

11 6 0 0.688012 0.260237 -4.246725

12 6 0 2.460617 0.030349 2.456418

13 6 0 1.095345 0.093019 2.878729

14 6 0 0.688012 0.260237 4.246725

15 6 0 -0.688006 0.260160 4.246735

16 6 0 -1.095337 0.092919 2.878737

17 7 0 0.000010 0.008036 2.056258

18 6 0 -2.460591 0.030105 2.456417

19 6 0 -2.898166 -0.003822 1.142159

20 6 0 -4.259368 -0.134719 0.680973

21 6 0 -4.259368 -0.134719 -0.680973

22 6 0 -2.898166 -0.003822 -1.142159

23 7 0 -2.116796 0.065207 -0.000000

24 6 0 -2.460591 0.030105 -2.456417

25 6 0 3.506136 -0.004787 -3.521267

26 6 0 4.428151 1.039796 -3.663420

27 6 0 5.405947 1.000053 -4.656136

28 6 0 5.476895 -0.086286 -5.526350

29 6 0 4.562218 -1.131781 -5.397404

30 6 0 3.585532 -1.089030 -4.405849

31 6 0 5.476895 -0.086286 5.526350

32 6 0 5.405947 1.000053 4.656136

33 6 0 4.428151 1.039796 3.663420

34 6 0 3.506136 -0.004787 3.521267

35 6 0 3.585532 -1.089030 4.405849

36 6 0 4.562218 -1.131781 5.397404

37 6 0 -3.506151 -0.004824 -3.521257

38 6 0 -3.585784 -1.089049 -4.405835

39 6 0 -4.562477 -1.131574 -5.397396

40 6 0 -5.476922 -0.085876 -5.526328

41 6 0 -5.405745 1.000438 -4.656102

42 6 0 -4.427943 1.039954 -3.663381

43 6 0 -3.506151 -0.004824 3.521257

44 6 0 -3.585784 -1.089049 4.405835

45 6 0 -4.562477 -1.131574 5.397396

46 6 0 -5.476922 -0.085876 5.526328

47 6 0 -5.405745 1.000438 4.656102

48 6 0 -4.427943 1.039954 3.663381

49 1 0 5.117581 -0.228244 1.327639

50 1 0 5.117581 -0.228244 -1.327639

51 1 0 -1.341880 0.375915 -5.098458

52 1 0 1.341887 0.376068 -5.098438

53 1 0 1.341887 0.376068 5.098438

54 1 0 -1.341880 0.375915 5.098458

55 1 0 -5.117530 -0.228785 1.327649

56 1 0 -5.117530 -0.228785 -1.327649

57 1 0 4.372588 1.891261 -2.993633

58 1 0 6.109312 1.821047 -4.751345

59 1 0 6.237718 -0.118511 -6.299335

60 1 0 4.611711 -1.983913 -6.067662

61 1 0 2.879424 -1.906396 -4.307408

62 1 0 6.237718 -0.118511 6.299335

63 1 0 6.109312 1.821047 4.751345

64 1 0 4.372588 1.891261 2.993633

65 1 0 2.879424 -1.906396 4.307408

66 1 0 4.611711 -1.983913 6.067662

67 1 0 -2.879853 -1.906568 -4.307396

68 1 0 -4.612165 -1.983687 -6.067664

69 1 0 -6.237750 -0.117925 -6.299317

70 1 0 -6.108933 1.821584 -4.751309

71 1 0 -4.372186 1.891401 -2.993590

72 1 0 -2.879853 -1.906568 4.307396

73 1 0 -4.612165 -1.983687 6.067664

74 1 0 -6.237750 -0.117925 6.299317

75 1 0 -6.108933 1.821584 4.751309

76 1 0 -4.372186 1.891401 2.993590

77 1 0 1.106606 0.094590 0.000000

78 1 0 -1.106605 0.095429 -0.000000

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

Rotational constants (GHZ): 0.0583453 0.0578427 0.0300215

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(Enter /home/kira/g09/l301.exe)

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

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

There are 513 symmetry adapted cartesian basis functions of A' symmetry.

There are 489 symmetry adapted cartesian basis functions of A" symmetry.

There are 488 symmetry adapted basis functions of A' symmetry.

There are 466 symmetry adapted basis functions of A" symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 161 beta electrons

nuclear repulsion energy 5346.0884616316 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= 78 NActive= 78 NUniq= 41 SFac= 3.62D+00 NAtFMM= 60 NAOKFM=T 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= -0.2116712628 Hartrees.

Nuclear repulsion after empirical dispersion term = 5345.8767903688 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= 78.

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

Smoothing algorithm: York/Karplus (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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5700

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.26D-11

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 268

GePol: Fraction of low-weight points (<1% of avg) = 4.70%

GePol: Cavity surface area = 617.928 Ang\*\*2

GePol: Cavity volume = 629.277 Ang\*\*3

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

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PCM non-electrostatic energy = -0.0019865784 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5345.8748037904 Hartrees.

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(Enter /home/kira/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.

One-electron integral symmetry used in STVInt

NBasis= 954 RedAO= T EigKep= 8.98D-05 NBF= 488 466

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 488 466

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= 938 938 939 939 940 MxSgAt= 78 MxSgA2= 78.

Leave Link 302 at Sun Aug 18 14:52:23 2019, MaxMem= 2013265920 cpu: 10.2

(Enter /home/kira/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sun Aug 18 14:52:24 2019, MaxMem= 2013265920 cpu: 1.2

(Enter /home/kira/g09/l401.exe)

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

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 -0.000000 -0.000005 Ang= -0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

Occupied (A') (A') (A") (A') (A') (A") (A') (A") (A") (A')

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The electronic state of the initial guess is 2-A'.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7586 S= 0.5043

Leave Link 401 at Sun Aug 18 14:52:28 2019, MaxMem= 2013265920 cpu: 31.6

(Enter /home/kira/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3047318 IEndB= 3047318 NGot= 2013265920 MDV= 2011240249

LenX= 2011240249 LenY= 2010235243

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= 480000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 97470000.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.33D-15 for 5686.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.74D-15 for 2692 215.

Iteration 1 A^-1\*A deviation from unit magnitude is 4.88D-15 for 5669.

Iteration 1 A^-1\*A deviation from orthogonality is 5.61D-08 for 5190 5145.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.66D-15 for 2616.

Iteration 2 A\*A^-1 deviation from orthogonality is 2.52D-15 for 2692 215.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 626.

Iteration 2 A^-1\*A deviation from orthogonality is 3.60D-16 for 4012 2907.

E= -1914.49355239846

DIIS: error= 2.96D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.49355239846 IErMin= 1 ErrMin= 2.96D-04

ErrMax= 2.96D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.47D-04 BMatP= 1.47D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 2.96D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.446 Goal= None Shift= 0.000

Gap= 0.504 Goal= None Shift= 0.000

RMSDP=8.79D-06 MaxDP=3.38D-04 OVMax= 1.47D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 8.79D-06 CP: 1.00D+00

E= -1914.49362587010 Delta-E= -0.000073471640 Rises=F Damp=F

DIIS: error= 4.04D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.49362587010 IErMin= 2 ErrMin= 4.04D-05

ErrMax= 4.04D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.75D-06 BMatP= 1.47D-04

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

Coeff-Com: -0.681D-01 0.107D+01

Coeff: -0.681D-01 0.107D+01

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=1.46D-06 MaxDP=6.04D-05 DE=-7.35D-05 OVMax= 2.24D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.31D-06 CP: 1.00D+00 1.07D+00

E= -1914.49362700284 Delta-E= -0.000001132733 Rises=F Damp=F

DIIS: error= 7.73D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.49362700284 IErMin= 3 ErrMin= 7.73D-06

ErrMax= 7.73D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.01D-07 BMatP= 1.75D-06

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

Coeff-Com: -0.216D-01 0.257D+00 0.765D+00

Coeff: -0.216D-01 0.257D+00 0.765D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=4.37D-07 MaxDP=1.78D-05 DE=-1.13D-06 OVMax= 6.79D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 3.73D-07 CP: 1.00D+00 1.09D+00 8.65D-01

E= -1914.49362703289 Delta-E= -0.000000030056 Rises=F Damp=F

DIIS: error= 6.87D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.49362703289 IErMin= 4 ErrMin= 6.87D-06

ErrMax= 6.87D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.07D-07 BMatP= 2.01D-07

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

Coeff-Com: -0.735D-02 0.681D-01 0.428D+00 0.512D+00

Coeff: -0.735D-02 0.681D-01 0.428D+00 0.512D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=2.43D-07 MaxDP=1.49D-05 DE=-3.01D-08 OVMax= 5.29D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.72D-07 CP: 1.00D+00 1.09D+00 9.19D-01 5.88D-01

E= -1914.49362705552 Delta-E= -0.000000022629 Rises=F Damp=F

DIIS: error= 3.03D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.49362705552 IErMin= 5 ErrMin= 3.03D-06

ErrMax= 3.03D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.33D-08 BMatP= 1.07D-07

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

Coeff-Com: 0.510D-03-0.180D-01 0.682D-01 0.281D+00 0.668D+00

Coeff: 0.510D-03-0.180D-01 0.682D-01 0.281D+00 0.668D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=9.54D-08 MaxDP=6.13D-06 DE=-2.26D-08 OVMax= 1.98D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 4.02D-08 CP: 1.00D+00 1.09D+00 9.29D-01 7.23D-01 6.08D-01

E= -1914.49362705830 Delta-E= -0.000000002784 Rises=F Damp=F

DIIS: error= 8.75D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.49362705830 IErMin= 6 ErrMin= 8.75D-07

ErrMax= 8.75D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.92D-09 BMatP= 1.33D-08

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

Coeff-Com: 0.765D-03-0.152D-01 0.141D-01 0.139D+00 0.408D+00 0.454D+00

Coeff: 0.765D-03-0.152D-01 0.141D-01 0.139D+00 0.408D+00 0.454D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=2.71D-08 MaxDP=1.65D-06 DE=-2.78D-09 OVMax= 4.98D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.04D-08 CP: 1.00D+00 1.09D+00 9.34D-01 7.05D-01 6.79D-01

CP: 5.17D-01

E= -1914.49362705870 Delta-E= -0.000000000397 Rises=F Damp=F

DIIS: error= 8.57D-08 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.49362705870 IErMin= 7 ErrMin= 8.57D-08

ErrMax= 8.57D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.02D-11 BMatP= 1.92D-09

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

Coeff-Com: 0.257D-03-0.469D-02 0.110D-02 0.369D-01 0.119D+00 0.171D+00

Coeff-Com: 0.676D+00

Coeff: 0.257D-03-0.469D-02 0.110D-02 0.369D-01 0.119D+00 0.171D+00

Coeff: 0.676D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=4.52D-09 MaxDP=2.31D-07 DE=-3.97D-10 OVMax= 8.11D-07

Error on total polarization charges = 0.08609

SCF Done: E(UB3LYP) = -1914.49362706 A.U. after 7 cycles

NFock= 7 Conv=0.45D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7586 S= 0.5043

<L.S>= 0.000000000000E+00

KE= 1.906564305848D+03 PE=-1.517669238459D+04 EE= 6.009759647895D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.25

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7586, after 0.7500

Leave Link 502 at Sun Aug 18 14:56:32 2019, MaxMem= 2013265920 cpu: 1937.9

(Enter /home/kira/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 = 179

Leave Link 701 at Sun Aug 18 14:56:47 2019, MaxMem= 2013265920 cpu: 124.4

(Enter /home/kira/g09/l702.exe)

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

Leave Link 702 at Sun Aug 18 14:56:47 2019, MaxMem= 2013265920 cpu: 0.2

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 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= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

Petite list used in FoFCou.

Leave Link 703 at Sun Aug 18 14:57:53 2019, MaxMem= 2013265920 cpu: 520.7

(Enter /home/kira/g09/l716.exe)

Dipole =-2.15031025D-04-1.17444912D-01-6.28830321D-13

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000033387 0.000030276 -0.000063279

2 6 -0.000040711 0.000013578 0.000059492

3 7 -0.000031596 -0.000153899 -0.000000000

4 6 -0.000040711 0.000013578 -0.000059492

5 6 0.000033387 0.000030276 0.000063279

6 6 0.000015950 0.000008650 0.000036363

7 6 -0.000029789 0.000056787 0.000029266

8 7 -0.000000510 -0.000090329 0.000004449

9 6 0.000031745 0.000051379 0.000029550

10 6 0.000013303 -0.000018398 -0.000012063

11 6 -0.000015047 -0.000021634 -0.000015813

12 6 0.000015950 0.000008650 -0.000036363

13 6 -0.000029789 0.000056787 -0.000029266

14 6 -0.000015047 -0.000021634 0.000015813

15 6 0.000013303 -0.000018398 0.000012063

16 6 0.000031745 0.000051379 -0.000029550

17 7 -0.000000510 -0.000090329 -0.000004449

18 6 -0.000022169 0.000010534 -0.000035450

19 6 0.000040739 0.000014083 0.000063011

20 6 -0.000029655 0.000022704 -0.000058419

21 6 -0.000029655 0.000022704 0.000058419

22 6 0.000040739 0.000014083 -0.000063011

23 7 0.000030710 -0.000118518 0.000000000

24 6 -0.000022169 0.000010534 0.000035450

25 6 -0.000029979 -0.000017646 0.000025867

26 6 0.000020567 0.000006169 -0.000019809

27 6 -0.000001593 0.000001795 0.000015108

28 6 0.000002620 -0.000005411 -0.000011291

29 6 0.000003133 0.000003840 -0.000005315

30 6 0.000002414 0.000009134 -0.000004666

31 6 0.000002620 -0.000005411 0.000011291

32 6 -0.000001593 0.000001795 -0.000015108

33 6 0.000020567 0.000006169 0.000019809

34 6 -0.000029979 -0.000017646 -0.000025867

35 6 0.000002414 0.000009134 0.000004666

36 6 0.000003133 0.000003840 0.000005315

37 6 0.000035676 -0.000019203 0.000030764

38 6 -0.000002777 0.000011285 -0.000005595

39 6 -0.000002966 0.000003585 -0.000003728

40 6 -0.000003827 -0.000005148 -0.000012305

41 6 0.000001957 0.000001585 0.000015823

42 6 -0.000020258 0.000006653 -0.000022059

43 6 0.000035676 -0.000019203 -0.000030764

44 6 -0.000002777 0.000011285 0.000005595

45 6 -0.000002966 0.000003585 0.000003728

46 6 -0.000003827 -0.000005148 0.000012305

47 6 0.000001957 0.000001585 -0.000015823

48 6 -0.000020258 0.000006653 0.000022059

49 1 0.000004898 -0.000012322 -0.000002388

50 1 0.000004898 -0.000012322 0.000002388

51 1 0.000000028 0.000002230 -0.000007580

52 1 -0.000001262 0.000001528 -0.000007188

53 1 -0.000001262 0.000001528 0.000007188

54 1 0.000000028 0.000002230 0.000007580

55 1 -0.000006212 -0.000010913 -0.000001595

56 1 -0.000006212 -0.000010913 0.000001595

57 1 -0.000002966 0.000001060 -0.000005422

58 1 0.000000531 0.000000962 -0.000000264

59 1 -0.000000200 0.000000479 0.000000088

60 1 -0.000000918 -0.000001384 0.000000071

61 1 0.000003060 -0.000001722 -0.000001228

62 1 -0.000000200 0.000000479 -0.000000088

63 1 0.000000531 0.000000962 0.000000264

64 1 -0.000002966 0.000001060 0.000005422

65 1 0.000003060 -0.000001722 0.000001228

66 1 -0.000000918 -0.000001384 -0.000000071

67 1 -0.000001831 -0.000002240 -0.000001482

68 1 0.000001480 -0.000001604 0.000000077

69 1 0.000000459 0.000000500 0.000000203

70 1 -0.000000692 0.000000982 0.000000239

71 1 0.000002456 0.000001199 -0.000004081

72 1 -0.000001831 -0.000002240 0.000001482

73 1 0.000001480 -0.000001604 -0.000000077

74 1 0.000000459 0.000000500 -0.000000203

75 1 -0.000000692 0.000000982 -0.000000239

76 1 0.000002456 0.000001199 0.000004081

77 1 -0.000008859 0.000094807 -0.000000000

78 1 0.000007660 0.000071563 0.000000000

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

Cartesian Forces: Max 0.000153899 RMS 0.000026121

Leave Link 716 at Sun Aug 18 14:57:53 2019, MaxMem= 2013265920 cpu: 0.2

(Enter /home/kira/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 0.000051216 RMS 0.000011766

Search for a local minimum.

Step number 9 out of a maximum of 452

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

RMS Force = .11766D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 3 4 5 6 7

8 9

DE= -2.09D-06 DEPred=-1.69D-06 R= 1.24D+00

TightC=F SS= 1.41D+00 RLast= 1.40D-02 DXNew= 1.6128D+00 4.1975D-02

Trust test= 1.24D+00 RLast= 1.40D-02 DXMaxT set to 9.59D-01

ITU= 1 1 1 0 1 1 1 1 0

Eigenvalues --- 0.00494 0.00815 0.00983 0.00988 0.00995

Eigenvalues --- 0.01525 0.01616 0.01622 0.01625 0.01635

Eigenvalues --- 0.01659 0.01723 0.01723 0.01723 0.01730

Eigenvalues --- 0.01737 0.01751 0.01773 0.01778 0.01792

Eigenvalues --- 0.01837 0.01847 0.01852 0.01856 0.01891

Eigenvalues --- 0.01903 0.01929 0.01939 0.01943 0.01983

Eigenvalues --- 0.02011 0.02020 0.02027 0.02030 0.02068

Eigenvalues --- 0.02069 0.02070 0.02071 0.02074 0.02092

Eigenvalues --- 0.02105 0.02118 0.02118 0.02119 0.02125

Eigenvalues --- 0.02130 0.02130 0.02132 0.02132 0.02132

Eigenvalues --- 0.02139 0.02160 0.02160 0.02160 0.02161

Eigenvalues --- 0.02162 0.02162 0.02162 0.02173 0.02173

Eigenvalues --- 0.02173 0.02175 0.02181 0.02181 0.02181

Eigenvalues --- 0.02184 0.02186 0.02187 0.02187 0.02189

Eigenvalues --- 0.02216 0.02217 0.02281 0.02729 0.04144

Eigenvalues --- 0.15921 0.15938 0.15942 0.15973 0.15997

Eigenvalues --- 0.15997 0.15997 0.15997 0.15998 0.15999

Eigenvalues --- 0.15999 0.15999 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16004 0.16014 0.16032

Eigenvalues --- 0.21952 0.22000 0.22000 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22005 0.22141 0.22759

Eigenvalues --- 0.22774 0.22816 0.22837 0.23472 0.23472

Eigenvalues --- 0.23477 0.23543 0.23853 0.24453 0.24734

Eigenvalues --- 0.24851 0.24866 0.24883 0.24974 0.24997

Eigenvalues --- 0.24997 0.24999 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25001 0.25098

Eigenvalues --- 0.25982 0.27973 0.34159 0.34180 0.34206

Eigenvalues --- 0.34576 0.35408 0.35413 0.35413 0.35413

Eigenvalues --- 0.35415 0.35415 0.35416 0.35416 0.35416

Eigenvalues --- 0.35416 0.35416 0.35420 0.35506 0.35507

Eigenvalues --- 0.35508 0.35522 0.35542 0.35545 0.35547

Eigenvalues --- 0.35704 0.36056 0.36057 0.36058 0.36106

Eigenvalues --- 0.36250 0.36251 0.36251 0.36276 0.37119

Eigenvalues --- 0.37159 0.37264 0.37294 0.37759 0.39130

Eigenvalues --- 0.39745 0.39986 0.40261 0.40421 0.40464

Eigenvalues --- 0.40804 0.41778 0.41781 0.41797 0.41982

Eigenvalues --- 0.42091 0.42093 0.42095 0.42146 0.42643

Eigenvalues --- 0.43275 0.44661 0.45285 0.45538 0.45569

Eigenvalues --- 0.45579 0.45586 0.45707 0.45773 0.45861

Eigenvalues --- 0.45890 0.45930 0.45941 0.45942 0.45948

Eigenvalues --- 0.45970 0.46610 0.46660 0.46660 0.46661

Eigenvalues --- 0.47073 0.47078 0.47086 0.47511 0.47608

Eigenvalues --- 0.48191 0.48279 0.49335 0.49434 0.49975

Eigenvalues --- 0.50744 0.50811 0.55296

En-DIIS/RFO-DIIS IScMMF= 0 using points: 9 8 7 6 5

RFO step: Lambda=-2.43250666D-07.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 4.29D-05 SmlDif= 1.00D-05

RMS Error= 0.6658389336D-04 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.29258 0.10974 -0.25804 -0.14469 0.00042

Iteration 1 RMS(Cart)= 0.00230742 RMS(Int)= 0.00000329

Iteration 2 RMS(Cart)= 0.00000271 RMS(Int)= 0.00000314

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000314

ITry= 1 IFail=0 DXMaxC= 9.46D-03 DCOld= 1.00D+10 DXMaxT= 9.59D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 4.87D-09 for atom 50.

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

(Linear) (Quad) (Total)

R1 2.72716 0.00004 0.00007 0.00005 0.00012 2.72728

R2 2.57371 -0.00005 -0.00001 -0.00008 -0.00008 2.57363

R3 2.03835 0.00000 -0.00002 0.00003 0.00001 2.03836

R4 2.61839 0.00002 0.00005 -0.00005 0.00000 2.61840

R5 2.61840 -0.00004 -0.00010 0.00001 -0.00009 2.61831

R6 2.61839 0.00002 0.00005 -0.00005 0.00000 2.61840

R7 1.90984 0.00001 -0.00006 0.00004 -0.00002 1.90982

R8 2.72716 0.00004 0.00007 0.00005 0.00012 2.72728

R9 2.61840 -0.00004 -0.00010 0.00001 -0.00009 2.61831

R10 2.03835 0.00000 -0.00002 0.00003 0.00001 2.03836

R11 2.70319 -0.00001 -0.00009 0.00000 -0.00009 2.70311

R12 2.82085 0.00000 0.00012 -0.00003 0.00009 2.82095

R13 2.59343 -0.00001 0.00017 -0.00012 0.00005 2.59348

R14 2.71575 0.00002 0.00002 0.00001 0.00003 2.71578

R15 2.59345 -0.00002 0.00016 -0.00011 0.00004 2.59349

R16 2.71576 0.00001 0.00004 -0.00003 0.00001 2.71577

R17 2.70318 -0.00001 -0.00004 -0.00005 -0.00009 2.70309

R18 2.60030 -0.00003 -0.00001 -0.00006 -0.00006 2.60023

R19 2.04089 0.00001 -0.00001 0.00003 0.00003 2.04092

R20 2.04089 0.00001 0.00000 0.00002 0.00002 2.04091

R21 2.70319 -0.00001 -0.00009 0.00000 -0.00009 2.70311

R22 2.82085 0.00000 0.00012 -0.00003 0.00009 2.82095

R23 2.71575 0.00002 0.00002 0.00001 0.00003 2.71578

R24 2.59343 -0.00001 0.00017 -0.00012 0.00005 2.59348

R25 2.60030 -0.00003 -0.00001 -0.00006 -0.00006 2.60023

R26 2.04089 0.00001 0.00000 0.00002 0.00002 2.04091

R27 2.71576 0.00001 0.00004 -0.00003 0.00001 2.71577

R28 2.04089 0.00001 -0.00001 0.00003 0.00003 2.04092

R29 2.59345 -0.00002 0.00016 -0.00011 0.00004 2.59349

R30 2.70318 -0.00001 -0.00004 -0.00005 -0.00009 2.70309

R31 2.61841 -0.00005 -0.00006 -0.00006 -0.00012 2.61829

R32 2.82089 -0.00001 0.00015 -0.00009 0.00005 2.82094

R33 2.72717 0.00004 0.00008 0.00003 0.00011 2.72728

R34 2.61837 0.00001 0.00009 -0.00007 0.00002 2.61838

R35 2.57370 -0.00005 -0.00003 -0.00006 -0.00009 2.57362

R36 2.03835 0.00000 -0.00003 0.00005 0.00001 2.03836

R37 2.72717 0.00004 0.00008 0.00003 0.00011 2.72728

R38 2.03835 0.00000 -0.00003 0.00005 0.00001 2.03836

R39 2.61837 0.00001 0.00009 -0.00007 0.00002 2.61838

R40 2.61841 -0.00005 -0.00006 -0.00006 -0.00012 2.61829

R41 1.90984 0.00001 -0.00004 0.00002 -0.00002 1.90982

R42 2.82089 -0.00001 0.00015 -0.00009 0.00005 2.82094

R43 2.64661 0.00002 0.00004 0.00003 0.00008 2.64669

R44 2.64857 0.00001 -0.00006 0.00002 -0.00004 2.64853

R45 2.63422 -0.00000 -0.00004 0.00002 -0.00002 2.63420

R46 2.04989 -0.00000 0.00001 -0.00002 -0.00001 2.04988

R47 2.63374 0.00001 0.00003 0.00000 0.00003 2.63377

R48 2.05087 0.00000 0.00001 -0.00000 0.00000 2.05087

R49 2.63637 -0.00000 -0.00002 -0.00001 -0.00003 2.63634

R50 2.05050 -0.00000 0.00001 -0.00000 0.00000 2.05051

R51 2.63135 0.00001 -0.00002 0.00006 0.00004 2.63140

R52 2.05088 0.00000 0.00001 -0.00000 0.00000 2.05088

R53 2.04961 -0.00000 0.00003 -0.00002 0.00001 2.04961

R54 2.63374 0.00001 0.00003 0.00000 0.00003 2.63377

R55 2.63637 -0.00000 -0.00002 -0.00001 -0.00003 2.63634

R56 2.05050 -0.00000 0.00001 -0.00000 0.00000 2.05051

R57 2.63422 -0.00000 -0.00004 0.00002 -0.00002 2.63420

R58 2.05087 0.00000 0.00001 -0.00000 0.00000 2.05087

R59 2.64661 0.00002 0.00004 0.00003 0.00008 2.64669

R60 2.04989 -0.00000 0.00001 -0.00002 -0.00001 2.04988

R61 2.64857 0.00001 -0.00006 0.00002 -0.00004 2.64853

R62 2.63135 0.00001 -0.00002 0.00006 0.00004 2.63140

R63 2.04961 -0.00000 0.00003 -0.00002 0.00001 2.04961

R64 2.05088 0.00000 0.00001 -0.00000 0.00000 2.05088

R65 2.64856 0.00000 -0.00004 0.00000 -0.00004 2.64852

R66 2.64660 0.00002 0.00006 0.00002 0.00008 2.64668

R67 2.63136 0.00001 -0.00002 0.00006 0.00004 2.63140

R68 2.04960 0.00000 0.00002 -0.00001 0.00001 2.04961

R69 2.63637 -0.00000 -0.00002 -0.00001 -0.00002 2.63634

R70 2.05088 0.00000 0.00001 -0.00000 0.00001 2.05088

R71 2.63374 0.00001 0.00002 0.00001 0.00003 2.63377

R72 2.05050 -0.00000 0.00001 -0.00000 0.00000 2.05051

R73 2.63422 -0.00001 -0.00004 0.00001 -0.00003 2.63420

R74 2.05087 0.00000 0.00001 -0.00000 0.00000 2.05087

R75 2.04989 -0.00000 0.00000 -0.00001 -0.00000 2.04988

R76 2.64856 0.00000 -0.00004 0.00000 -0.00004 2.64852

R77 2.64660 0.00002 0.00006 0.00002 0.00008 2.64668

R78 2.63136 0.00001 -0.00002 0.00006 0.00004 2.63140

R79 2.04960 0.00000 0.00002 -0.00001 0.00001 2.04961

R80 2.63637 -0.00000 -0.00002 -0.00001 -0.00002 2.63634

R81 2.05088 0.00000 0.00001 -0.00000 0.00001 2.05088

R82 2.63374 0.00001 0.00002 0.00001 0.00003 2.63377

R83 2.05050 -0.00000 0.00001 -0.00000 0.00000 2.05051

R84 2.63422 -0.00001 -0.00004 0.00001 -0.00003 2.63420

R85 2.05087 0.00000 0.00001 -0.00000 0.00000 2.05087

R86 2.04989 -0.00000 0.00000 -0.00001 -0.00000 2.04988

A1 1.89607 0.00001 0.00004 -0.00002 0.00002 1.89609

A2 2.17334 0.00000 0.00005 0.00001 0.00005 2.17340

A3 2.21369 -0.00001 -0.00009 0.00001 -0.00008 2.21361

A4 1.84731 0.00000 -0.00010 0.00004 -0.00006 1.84726

A5 2.21830 0.00000 0.00001 0.00000 0.00002 2.21832

A6 2.21750 -0.00001 0.00010 -0.00004 0.00004 2.21755

A7 1.93798 -0.00001 0.00012 -0.00005 0.00006 1.93804

A8 2.17136 0.00001 0.00009 0.00011 0.00018 2.17154

A9 2.17136 0.00001 0.00009 0.00011 0.00018 2.17154

A10 1.84731 0.00000 -0.00010 0.00004 -0.00006 1.84726

A11 2.21750 -0.00001 0.00010 -0.00004 0.00004 2.21755

A12 2.21830 0.00000 0.00001 0.00000 0.00002 2.21832

A13 1.89607 0.00001 0.00004 -0.00002 0.00002 1.89609

A14 2.21369 -0.00001 -0.00009 0.00001 -0.00008 2.21361

A15 2.17334 0.00000 0.00005 0.00001 0.00005 2.17340

A16 2.19261 -0.00001 -0.00005 0.00002 -0.00004 2.19257

A17 2.04301 0.00002 -0.00006 0.00006 0.00000 2.04301

A18 2.04757 -0.00001 0.00011 -0.00007 0.00004 2.04761

A19 2.19211 -0.00000 0.00005 -0.00009 -0.00005 2.19206

A20 2.16114 -0.00002 0.00006 -0.00007 0.00001 2.16114

A21 1.92993 0.00002 -0.00011 0.00016 0.00005 1.92998

A22 1.84836 -0.00003 0.00009 -0.00020 -0.00010 1.84826

A23 1.92992 0.00002 -0.00013 0.00020 0.00007 1.93000

A24 2.19210 -0.00000 0.00002 -0.00006 -0.00005 2.19205

A25 2.16116 -0.00002 0.00012 -0.00015 -0.00002 2.16114

A26 1.85817 -0.00001 0.00008 -0.00010 -0.00001 1.85816

A27 2.20381 0.00001 0.00010 0.00005 0.00015 2.20396

A28 2.22112 -0.00000 -0.00019 0.00005 -0.00014 2.22098

A29 1.85817 -0.00001 0.00007 -0.00006 0.00001 1.85818

A30 2.20380 0.00001 0.00009 0.00005 0.00014 2.20394

A31 2.22112 -0.00000 -0.00016 0.00001 -0.00015 2.22097

A32 2.19261 -0.00001 -0.00005 0.00002 -0.00004 2.19257

A33 2.04301 0.00002 -0.00006 0.00006 0.00000 2.04301

A34 2.04757 -0.00001 0.00011 -0.00007 0.00004 2.04761

A35 2.16114 -0.00002 0.00006 -0.00007 0.00001 2.16114

A36 2.19211 -0.00000 0.00005 -0.00009 -0.00005 2.19206

A37 1.92993 0.00002 -0.00011 0.00016 0.00005 1.92998

A38 1.85817 -0.00001 0.00007 -0.00006 0.00001 1.85818

A39 2.20380 0.00001 0.00009 0.00005 0.00014 2.20394

A40 2.22112 -0.00000 -0.00016 0.00001 -0.00015 2.22097

A41 1.85817 -0.00001 0.00008 -0.00010 -0.00001 1.85816

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A46 2.19210 -0.00000 0.00002 -0.00006 -0.00005 2.19205

A47 1.84836 -0.00003 0.00009 -0.00020 -0.00010 1.84826

A48 2.19261 -0.00001 -0.00007 0.00005 -0.00004 2.19257

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A54 1.89607 0.00000 0.00006 -0.00004 0.00002 1.89609

A55 2.17333 0.00000 0.00005 0.00001 0.00006 2.17339

A56 2.21370 -0.00001 -0.00011 0.00002 -0.00009 2.21362

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A74 2.09212 -0.00001 -0.00002 0.00000 -0.00002 2.09210

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A76 2.08923 -0.00000 0.00004 -0.00001 0.00003 2.08926

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D2 3.13402 0.00001 0.00095 0.00028 0.00122 3.13524

D3 -3.12443 0.00001 0.00108 0.00014 0.00122 -3.12321

D4 0.00525 0.00001 0.00133 0.00039 0.00172 0.00697

D5 -0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D6 -3.12839 0.00000 0.00040 0.00012 0.00052 -3.12788

D7 3.12839 -0.00000 -0.00040 -0.00012 -0.00052 3.12788

D8 0.00000 0.00000 0.00000 0.00000 -0.00000 0.00000

D9 -0.00726 -0.00001 -0.00116 -0.00004 -0.00120 -0.00846

D10 3.06129 0.00004 0.00283 0.00258 0.00542 3.06671

D11 -3.13694 -0.00001 -0.00141 -0.00029 -0.00170 -3.13865

D12 -0.06840 0.00003 0.00258 0.00233 0.00491 -0.06348

D13 -3.08256 -0.00000 -0.00017 -0.00047 -0.00064 -3.08319

D14 0.05667 -0.00000 -0.00032 -0.00010 -0.00043 0.05624

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D16 -3.09928 0.00001 -0.00002 0.00020 0.00018 -3.09910

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D29 -0.10933 -0.00001 0.00045 0.00004 0.00049 -0.10884

D30 3.02906 0.00000 0.00074 -0.00016 0.00059 3.02964

D31 3.02989 -0.00001 0.00030 0.00040 0.00070 3.03060

D32 -0.11491 0.00000 0.00059 0.00021 0.00080 -0.11411

D33 -1.12608 -0.00000 -0.00055 -0.00011 -0.00066 -1.12673

D34 2.01674 0.00000 -0.00051 -0.00000 -0.00051 2.01623

D35 2.01768 -0.00000 -0.00041 -0.00044 -0.00085 2.01683

D36 -1.12268 0.00000 -0.00037 -0.00034 -0.00071 -1.12339

D37 -3.12524 -0.00002 0.00010 -0.00063 -0.00052 -3.12576

D38 0.01920 -0.00003 -0.00016 -0.00045 -0.00061 0.01859

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D40 -0.02259 -0.00000 -0.00018 0.00021 0.00003 -0.02256

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D43 -0.01919 0.00003 0.00016 0.00039 0.00056 -0.01863

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D47 -3.13231 -0.00001 0.00018 -0.00044 -0.00026 -3.13257

D48 0.02260 0.00000 0.00021 -0.00024 -0.00003 0.02257

D49 0.10916 0.00001 -0.00046 0.00000 -0.00046 0.10870

D50 -3.03012 0.00001 -0.00032 -0.00036 -0.00069 -3.03081

D51 -3.02925 -0.00000 -0.00079 0.00029 -0.00050 -3.02975

D52 0.11465 -0.00000 -0.00066 -0.00007 -0.00073 0.11392

D53 0.00002 -0.00000 0.00001 -0.00009 -0.00008 -0.00006

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D66 0.02259 0.00000 0.00018 -0.00021 -0.00003 0.02256

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D69 3.12524 0.00002 -0.00010 0.00063 0.00052 3.12576

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D72 -3.12812 0.00001 0.00001 0.00029 0.00030 -3.12781

D73 3.12810 -0.00001 -0.00002 -0.00022 -0.00024 3.12786

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D77 3.11623 0.00001 0.00008 -0.00001 0.00007 3.11630

D78 -0.02260 -0.00000 -0.00021 0.00024 0.00003 -0.02257

D79 0.01919 -0.00003 -0.00016 -0.00039 -0.00056 0.01863

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D87 -0.05658 -0.00000 0.00023 0.00011 0.00034 -0.05624

D88 3.09937 -0.00001 -0.00016 -0.00015 -0.00031 3.09905

D89 -1.12301 0.00000 -0.00024 0.00002 -0.00023 -1.12324

D90 2.01734 -0.00000 -0.00030 -0.00007 -0.00037 2.01697

D91 2.01647 0.00000 -0.00037 0.00035 -0.00002 2.01645

D92 -1.12636 -0.00000 -0.00043 0.00026 -0.00016 -1.12652

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D94 -0.00559 -0.00001 -0.00134 -0.00026 -0.00160 -0.00718

D95 -0.00456 -0.00000 -0.00063 0.00000 -0.00062 -0.00519

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D97 3.13733 0.00001 0.00137 0.00021 0.00159 3.13892

D98 0.06631 -0.00003 -0.00183 -0.00173 -0.00356 0.06276

D99 0.00764 0.00001 0.00105 -0.00001 0.00104 0.00868

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D103 -3.12828 0.00000 0.00040 0.00004 0.00044 -3.12784

D104 0.00000 0.00000 0.00000 0.00000 -0.00000 0.00000

D105 0.00456 0.00000 0.00063 -0.00000 0.00062 0.00519

D106 3.13425 0.00001 0.00095 0.00022 0.00117 3.13542

D107 -3.12410 0.00001 0.00102 0.00004 0.00105 -3.12305

D108 0.00559 0.00001 0.00134 0.00026 0.00160 0.00718

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D113 -3.08271 0.00000 -0.00009 -0.00048 -0.00057 -3.08328

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D115 0.04453 0.00001 0.00030 -0.00021 0.00009 0.04461

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D178 -3.13340 -0.00000 -0.00011 0.00002 -0.00009 -3.13348

D179 3.13725 -0.00000 -0.00016 0.00009 -0.00007 3.13718

D180 -0.00024 -0.00000 -0.00014 0.00008 -0.00005 -0.00029

D181 -0.00012 0.00000 0.00009 -0.00006 0.00003 -0.00008

D182 3.14067 0.00000 0.00003 0.00001 0.00004 3.14071

D183 3.13736 0.00000 0.00007 -0.00005 0.00002 3.13737

D184 -0.00504 -0.00000 0.00001 0.00001 0.00002 -0.00502

D185 -0.00108 0.00000 -0.00001 0.00014 0.00013 -0.00095

D186 3.13581 -0.00000 0.00002 0.00001 0.00003 3.13584

D187 3.14132 0.00000 0.00005 0.00008 0.00012 3.14144

D188 -0.00498 -0.00000 0.00008 -0.00005 0.00003 -0.00495

D189 -0.00168 -0.00000 -0.00003 -0.00019 -0.00022 -0.00189

D190 3.13337 -0.00000 -0.00015 0.00001 -0.00014 3.13323

D191 -3.13858 -0.00000 -0.00006 -0.00006 -0.00012 -3.13871

D192 -0.00353 -0.00000 -0.00018 0.00014 -0.00005 -0.00358

D193 -3.13608 -0.00000 -0.00015 -0.00001 -0.00016 -3.13625

D194 -0.00287 -0.00000 -0.00018 0.00005 -0.00013 -0.00300

D195 0.00671 0.00000 -0.00009 0.00007 -0.00002 0.00669

D196 3.13992 0.00000 -0.00012 0.00014 0.00002 3.13994

D197 3.13730 0.00000 0.00007 -0.00007 0.00000 3.13730

D198 -0.01080 0.00000 -0.00005 0.00013 0.00008 -0.01072

D199 -0.00550 -0.00000 0.00001 -0.00016 -0.00014 -0.00564

D200 3.12958 -0.00000 -0.00011 0.00004 -0.00007 3.12952

D201 -0.00409 0.00000 0.00013 -0.00002 0.00011 -0.00399

D202 3.13340 0.00000 0.00011 -0.00002 0.00009 3.13348

D203 -3.13725 0.00000 0.00016 -0.00009 0.00007 -3.13718

D204 0.00024 0.00000 0.00014 -0.00008 0.00005 0.00029

D205 0.00012 -0.00000 -0.00009 0.00006 -0.00003 0.00008

D206 -3.14067 -0.00000 -0.00003 -0.00001 -0.00004 -3.14071

D207 -3.13736 -0.00000 -0.00007 0.00005 -0.00002 -3.13737

D208 0.00504 0.00000 -0.00001 -0.00001 -0.00002 0.00502

D209 0.00108 -0.00000 0.00001 -0.00014 -0.00013 0.00095

D210 -3.13581 0.00000 -0.00002 -0.00001 -0.00003 -3.13584

D211 -3.14132 -0.00000 -0.00005 -0.00008 -0.00012 -3.14144

D212 0.00498 0.00000 -0.00008 0.00005 -0.00003 0.00495

D213 0.00168 0.00000 0.00003 0.00019 0.00022 0.00189

D214 -3.13337 0.00000 0.00015 -0.00001 0.00014 -3.13323

D215 3.13858 0.00000 0.00006 0.00006 0.00012 3.13871

D216 0.00353 0.00000 0.00018 -0.00014 0.00005 0.00358

Item Value Threshold Converged?

Maximum Force 0.000051 0.000450 YES

RMS Force 0.000012 0.000300 YES

Maximum Displacement 0.009465 0.001800 NO

RMS Displacement 0.002308 0.001200 NO

Predicted change in Energy=-9.435074D-07

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Aug 18 14:57:53 2019, MaxMem= 2013265920 cpu: 1.4

(Enter /home/kira/g09/l202.exe)

Stoichiometry C44H30N4(1-,2)

Framework group CS[SG(H2N2),X(C44H28N2)]

Deg. of freedom 116

Full point group CS NOp 2

RotChk: IX=3 Diff= 2.53D-05

Largest Abelian subgroup CS NOp 2

Largest concise Abelian subgroup CS NOp 2

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 4.259350 -0.136092 0.680952

2 6 0 2.898020 -0.006080 1.142190

3 7 0 2.116564 0.061787 0.000000

4 6 0 2.898020 -0.006080 -1.142190

5 6 0 4.259350 -0.136092 -0.680952

6 6 0 2.460557 0.028645 -2.456407

7 6 0 1.095324 0.091087 -2.878721

8 7 0 0.000009 0.005353 -2.056255

9 6 0 -1.095318 0.090982 -2.878721

10 6 0 -0.688011 0.258712 -4.246674

11 6 0 0.687973 0.258727 -4.246677

12 6 0 2.460557 0.028645 2.456407

13 6 0 1.095324 0.091087 2.878721

14 6 0 0.687973 0.258727 4.246677

15 6 0 -0.688011 0.258712 4.246674

16 6 0 -1.095318 0.090982 2.878721

17 7 0 0.000009 0.005353 2.056255

18 6 0 -2.460530 0.028386 2.456391

19 6 0 -2.897966 -0.006555 1.142181

20 6 0 -4.259295 -0.136628 0.680950

21 6 0 -4.259295 -0.136628 -0.680950

22 6 0 -2.897966 -0.006555 -1.142181

23 7 0 -2.116497 0.061168 -0.000000

24 6 0 -2.460530 0.028386 -2.456391

25 6 0 3.506238 -0.004720 -3.521222

26 6 0 4.427049 1.041083 -3.662605

27 6 0 5.405027 1.003232 -4.655201

28 6 0 5.477292 -0.082337 -5.526293

29 6 0 4.563821 -1.128972 -5.398202

30 6 0 3.587042 -1.088162 -4.406625

31 6 0 5.477292 -0.082337 5.526293

32 6 0 5.405027 1.003232 4.655201

33 6 0 4.427049 1.041083 3.662605

34 6 0 3.506238 -0.004720 3.521222

35 6 0 3.587042 -1.088162 4.406625

36 6 0 4.563821 -1.128972 5.398202

37 6 0 -3.506237 -0.004797 -3.521182

38 6 0 -3.586923 -1.087952 -4.406942

39 6 0 -4.563720 -1.128546 -5.398511

40 6 0 -5.477336 -0.081991 -5.526213

41 6 0 -5.405197 1.003287 -4.654747

42 6 0 -4.427189 1.040933 -3.662175

43 6 0 -3.506237 -0.004797 3.521182

44 6 0 -3.586923 -1.087952 4.406942

45 6 0 -4.563720 -1.128546 5.398511

46 6 0 -5.477336 -0.081991 5.526213

47 6 0 -5.405197 1.003287 4.654747

48 6 0 -4.427189 1.040933 3.662175

49 1 0 5.117601 -0.229954 1.327550

50 1 0 5.117601 -0.229954 -1.327550

51 1 0 -1.341779 0.375020 -5.098421

52 1 0 1.341722 0.375062 -5.098431

53 1 0 1.341722 0.375062 5.098431

54 1 0 -1.341779 0.375020 5.098421

55 1 0 -5.117533 -0.230557 1.327557

56 1 0 -5.117533 -0.230557 -1.327557

57 1 0 4.370366 1.892012 -2.992238

58 1 0 6.107453 1.825111 -4.749725

59 1 0 6.238187 -0.113070 -6.299272

60 1 0 4.614333 -1.980515 -6.069138

61 1 0 2.881928 -1.906471 -4.308852

62 1 0 6.238187 -0.113070 6.299272

63 1 0 6.107453 1.825111 4.749725

64 1 0 4.370366 1.892012 2.992238

65 1 0 2.881928 -1.906471 4.308852

66 1 0 4.614333 -1.980515 6.069138

67 1 0 -2.881697 -1.906201 -4.309467

68 1 0 -4.614133 -1.979859 -6.069746

69 1 0 -6.238251 -0.112562 -6.299179

70 1 0 -6.107751 1.825093 -4.748952

71 1 0 -4.370606 1.891634 -2.991510

72 1 0 -2.881697 -1.906201 4.309467

73 1 0 -4.614133 -1.979859 6.069746

74 1 0 -6.238251 -0.112562 6.299179

75 1 0 -6.107751 1.825093 4.748952

76 1 0 -4.370606 1.891634 2.991510

77 1 0 1.106440 0.093965 0.000000

78 1 0 -1.106396 0.093992 -0.000000

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

Rotational constants (GHZ): 0.0583430 0.0578437 0.0300208

Leave Link 202 at Sun Aug 18 14:57:53 2019, MaxMem= 2013265920 cpu: 0.1

(Enter /home/kira/g09/l301.exe)

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

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

There are 513 symmetry adapted cartesian basis functions of A' symmetry.

There are 489 symmetry adapted cartesian basis functions of A" symmetry.

There are 488 symmetry adapted basis functions of A' symmetry.

There are 466 symmetry adapted basis functions of A" symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 161 beta electrons

nuclear repulsion energy 5346.0710884431 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= 78 NActive= 78 NUniq= 41 SFac= 3.62D+00 NAtFMM= 60 NAOKFM=T 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= -0.2116685548 Hartrees.

Nuclear repulsion after empirical dispersion term = 5345.8594198883 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= 78.

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

Smoothing algorithm: York/Karplus (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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5706

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.18D-09

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 278

GePol: Fraction of low-weight points (<1% of avg) = 4.87%

GePol: Cavity surface area = 617.912 Ang\*\*2

GePol: Cavity volume = 629.236 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0019874876 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5345.8574324007 Hartrees.

Leave Link 301 at Sun Aug 18 14:57:53 2019, MaxMem= 2013265920 cpu: 1.0

(Enter /home/kira/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.

One-electron integral symmetry used in STVInt

NBasis= 954 RedAO= T EigKep= 8.98D-05 NBF= 488 466

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 488 466

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= 938 938 939 939 940 MxSgAt= 78 MxSgA2= 78.

Leave Link 302 at Sun Aug 18 14:57:54 2019, MaxMem= 2013265920 cpu: 10.6

(Enter /home/kira/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sun Aug 18 14:57:54 2019, MaxMem= 2013265920 cpu: 1.2

(Enter /home/kira/g09/l401.exe)

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

B after Tr= -0.000000 0.000000 -0.000000

Rot= 1.000000 0.000000 0.000000 -0.000006 Ang= -0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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The electronic state of the initial guess is 2-A'.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7586 S= 0.5043

Leave Link 401 at Sun Aug 18 14:57:59 2019, MaxMem= 2013265920 cpu: 33.2

(Enter /home/kira/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3047318 IEndB= 3047318 NGot= 2013265920 MDV= 2011240249

LenX= 2011240249 LenY= 2010235243

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= 480000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 97675308.

Iteration 1 A\*A^-1 deviation from unit magnitude is 4.88D-15 for 5703.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.77D-15 for 5703 159.

Iteration 1 A^-1\*A deviation from unit magnitude is 4.88D-15 for 5674.

Iteration 1 A^-1\*A deviation from orthogonality is 6.14D-08 for 4780 4773.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.66D-15 for 2570.

Iteration 2 A\*A^-1 deviation from orthogonality is 2.87D-15 for 4792 2570.

Iteration 2 A^-1\*A deviation from unit magnitude is 9.99D-16 for 2938.

Iteration 2 A^-1\*A deviation from orthogonality is 6.66D-16 for 5581 56.

E= -1914.49360601711

DIIS: error= 1.86D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.49360601711 IErMin= 1 ErrMin= 1.86D-04

ErrMax= 1.86D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.81D-05 BMatP= 5.81D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.86D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.446 Goal= None Shift= 0.000

Gap= 0.504 Goal= None Shift= 0.000

RMSDP=6.08D-06 MaxDP=3.99D-04 OVMax= 5.72D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 6.08D-06 CP: 1.00D+00

E= -1914.49362777937 Delta-E= -0.000021762266 Rises=F Damp=F

DIIS: error= 1.43D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.49362777937 IErMin= 2 ErrMin= 1.43D-05

ErrMax= 1.43D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.93D-07 BMatP= 5.81D-05

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

Coeff-Com: -0.582D-01 0.106D+01

Coeff: -0.582D-01 0.106D+01

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=7.53D-07 MaxDP=6.22D-05 DE=-2.18D-05 OVMax= 9.21D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 6.32D-07 CP: 1.00D+00 1.07D+00

E= -1914.49362795044 Delta-E= -0.000000171063 Rises=F Damp=F

DIIS: error= 6.86D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.49362795044 IErMin= 3 ErrMin= 6.86D-06

ErrMax= 6.86D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.42D-07 BMatP= 3.93D-07

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

Coeff-Com: -0.286D-01 0.459D+00 0.570D+00

Coeff: -0.286D-01 0.459D+00 0.570D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=2.54D-07 MaxDP=1.68D-05 DE=-1.71D-07 OVMax= 4.34D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.16D-07 CP: 1.00D+00 1.07D+00 7.96D-01

E= -1914.49362797845 Delta-E= -0.000000028017 Rises=F Damp=F

DIIS: error= 3.56D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.49362797845 IErMin= 4 ErrMin= 3.56D-06

ErrMax= 3.56D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.22D-08 BMatP= 1.42D-07

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

Coeff-Com: -0.546D-02 0.625D-01 0.322D+00 0.621D+00

Coeff: -0.546D-02 0.625D-01 0.322D+00 0.621D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=1.05D-07 MaxDP=5.94D-06 DE=-2.80D-08 OVMax= 1.79D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 6.68D-08 CP: 1.00D+00 1.07D+00 8.76D-01 7.15D-01

E= -1914.49362798628 Delta-E= -0.000000007826 Rises=F Damp=F

DIIS: error= 8.66D-07 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.49362798628 IErMin= 5 ErrMin= 8.66D-07

ErrMax= 8.66D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.94D-09 BMatP= 3.22D-08

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

Coeff-Com: -0.357D-03-0.477D-02 0.106D+00 0.285D+00 0.614D+00

Coeff: -0.357D-03-0.477D-02 0.106D+00 0.285D+00 0.614D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=3.91D-08 MaxDP=2.41D-06 DE=-7.83D-09 OVMax= 8.71D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.48D-08 CP: 1.00D+00 1.07D+00 8.78D-01 7.99D-01 6.51D-01

E= -1914.49362798665 Delta-E= -0.000000000372 Rises=F Damp=F

DIIS: error= 5.14D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.49362798665 IErMin= 6 ErrMin= 5.14D-07

ErrMax= 5.14D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.87D-10 BMatP= 1.94D-09

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

Coeff-Com: 0.476D-03-0.108D-01 0.251D-01 0.980D-01 0.389D+00 0.498D+00

Coeff: 0.476D-03-0.108D-01 0.251D-01 0.980D-01 0.389D+00 0.498D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=1.64D-08 MaxDP=1.07D-06 DE=-3.72D-10 OVMax= 4.05D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 6.32D-09 CP: 1.00D+00 1.07D+00 8.87D-01 7.83D-01 7.57D-01

CP: 5.41D-01

E= -1914.49362798681 Delta-E= -0.000000000156 Rises=F Damp=F

DIIS: error= 8.73D-08 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.49362798681 IErMin= 7 ErrMin= 8.73D-08

ErrMax= 8.73D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.03D-11 BMatP= 5.87D-10

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

Coeff-Com: 0.233D-03-0.455D-02 0.404D-02 0.245D-01 0.133D+00 0.224D+00

Coeff-Com: 0.619D+00

Coeff: 0.233D-03-0.455D-02 0.404D-02 0.245D-01 0.133D+00 0.224D+00

Coeff: 0.619D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=3.61D-09 MaxDP=2.16D-07 DE=-1.56D-10 OVMax= 7.13D-07

Error on total polarization charges = 0.08609

SCF Done: E(UB3LYP) = -1914.49362799 A.U. after 7 cycles

NFock= 7 Conv=0.36D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7586 S= 0.5043

<L.S>= 0.000000000000E+00

KE= 1.906563962436D+03 PE=-1.517665769668D+04 EE= 6.009742673855D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.25

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7586, after 0.7500

Leave Link 502 at Sun Aug 18 15:01:59 2019, MaxMem= 2013265920 cpu: 1907.4

(Enter /home/kira/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 = 179

Leave Link 701 at Sun Aug 18 15:02:15 2019, MaxMem= 2013265920 cpu: 124.5

(Enter /home/kira/g09/l702.exe)

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

Leave Link 702 at Sun Aug 18 15:02:15 2019, MaxMem= 2013265920 cpu: 0.1

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 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= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

Petite list used in FoFCou.

Leave Link 703 at Sun Aug 18 15:03:20 2019, MaxMem= 2013265920 cpu: 520.3

(Enter /home/kira/g09/l716.exe)

Dipole =-1.37065552D-04-1.06728467D-01 5.41788836D-13

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000007302 -0.000005111 -0.000025453

2 6 -0.000001842 0.000038370 -0.000003891

3 7 0.000000830 -0.000063181 -0.000000000

4 6 -0.000001842 0.000038370 0.000003891

5 6 0.000007302 -0.000005111 0.000025453

6 6 0.000035511 -0.000022748 -0.000000672

7 6 -0.000038486 0.000003337 0.000012885

8 7 -0.000000482 -0.000004995 -0.000051539

9 6 0.000038302 0.000009160 0.000018787

10 6 -0.000002106 0.000000520 -0.000007138

11 6 0.000010071 0.000009289 -0.000008727

12 6 0.000035511 -0.000022748 0.000000672

13 6 -0.000038486 0.000003337 -0.000012885

14 6 0.000010071 0.000009289 0.000008727

15 6 -0.000002106 0.000000520 0.000007138

16 6 0.000038302 0.000009160 -0.000018787

17 7 -0.000000482 -0.000004995 0.000051539

18 6 -0.000038827 -0.000022366 0.000009144

19 6 -0.000000924 0.000037346 -0.000009420

20 6 -0.000006084 -0.000008485 -0.000022622

21 6 -0.000006084 -0.000008485 0.000022622

22 6 -0.000000924 0.000037346 0.000009420

23 7 -0.000008249 -0.000047819 -0.000000000

24 6 -0.000038827 -0.000022366 -0.000009144

25 6 -0.000000976 0.000017713 0.000015028

26 6 0.000004597 -0.000006826 0.000003266

27 6 -0.000007064 -0.000000459 -0.000002799

28 6 0.000001931 0.000001717 0.000000524

29 6 -0.000001675 -0.000000026 -0.000000361

30 6 -0.000010663 -0.000008291 -0.000000121

31 6 0.000001931 0.000001717 -0.000000524

32 6 -0.000007064 -0.000000459 0.000002799

33 6 0.000004597 -0.000006826 -0.000003266

34 6 -0.000000976 0.000017713 -0.000015028

35 6 -0.000010663 -0.000008291 0.000000121

36 6 -0.000001675 -0.000000026 0.000000361

37 6 0.000004379 0.000018075 0.000018320

38 6 0.000008936 -0.000009412 -0.000002066

39 6 0.000001552 -0.000000312 0.000000007

40 6 -0.000002827 0.000001868 -0.000000015

41 6 0.000006856 -0.000000822 -0.000002793

42 6 -0.000008239 -0.000006045 0.000000453

43 6 0.000004379 0.000018075 -0.000018320

44 6 0.000008936 -0.000009412 0.000002066

45 6 0.000001552 -0.000000312 -0.000000007

46 6 -0.000002827 0.000001868 0.000000015

47 6 0.000006856 -0.000000822 0.000002793

48 6 -0.000008239 -0.000006045 -0.000000453

49 1 -0.000001448 0.000002204 0.000006568

50 1 -0.000001448 0.000002204 -0.000006568

51 1 -0.000004560 -0.000005121 0.000009087

52 1 0.000007620 -0.000004291 0.000006795

53 1 0.000007620 -0.000004291 -0.000006795

54 1 -0.000004560 -0.000005121 -0.000009087

55 1 0.000002260 0.000002543 0.000004390

56 1 0.000002260 0.000002543 -0.000004390

57 1 0.000001035 0.000002067 -0.000000181

58 1 -0.000002312 0.000001319 0.000002660

59 1 -0.000000677 0.000000538 0.000002202

60 1 -0.000003000 -0.000001460 0.000002847

61 1 0.000001243 -0.000001417 -0.000003463

62 1 -0.000000677 0.000000538 -0.000002202

63 1 -0.000002312 0.000001319 -0.000002660

64 1 0.000001035 0.000002067 0.000000181

65 1 0.000001243 -0.000001417 0.000003463

66 1 -0.000003000 -0.000001460 -0.000002847

67 1 -0.000002162 -0.000001163 -0.000003334

68 1 0.000002753 -0.000001927 0.000003269

69 1 0.000000863 0.000000591 0.000002213

70 1 0.000002826 0.000001808 0.000001893

71 1 -0.000000167 0.000001951 -0.000001506

72 1 -0.000002162 -0.000001163 0.000003334

73 1 0.000002753 -0.000001927 -0.000003269

74 1 0.000000863 0.000000591 -0.000002213

75 1 0.000002826 0.000001808 -0.000001893

76 1 -0.000000167 0.000001951 0.000001506

77 1 -0.000003742 0.000019724 -0.000000000

78 1 0.000004129 0.000012995 0.000000000

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

Cartesian Forces: Max 0.000063181 RMS 0.000013263

Leave Link 716 at Sun Aug 18 15:03:20 2019, MaxMem= 2013265920 cpu: 0.2

(Enter /home/kira/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 0.000033148 RMS 0.000006588

Search for a local minimum.

Step number 10 out of a maximum of 452

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

RMS Force = .65883D-05 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 3 4 5 6 7

8 9 10

DE= -9.28D-07 DEPred=-9.44D-07 R= 9.84D-01

Trust test= 9.84D-01 RLast= 1.50D-02 DXMaxT set to 9.59D-01

ITU= 0 1 1 1 0 1 1 1 1 0

Eigenvalues --- 0.00430 0.00827 0.00983 0.00988 0.00995

Eigenvalues --- 0.01549 0.01616 0.01625 0.01628 0.01635

Eigenvalues --- 0.01659 0.01723 0.01723 0.01723 0.01734

Eigenvalues --- 0.01737 0.01751 0.01769 0.01773 0.01792

Eigenvalues --- 0.01837 0.01844 0.01847 0.01856 0.01891

Eigenvalues --- 0.01904 0.01930 0.01943 0.01951 0.01983

Eigenvalues --- 0.02011 0.02020 0.02027 0.02068 0.02069

Eigenvalues --- 0.02070 0.02070 0.02074 0.02080 0.02093

Eigenvalues --- 0.02108 0.02118 0.02118 0.02119 0.02130

Eigenvalues --- 0.02130 0.02132 0.02132 0.02132 0.02134

Eigenvalues --- 0.02149 0.02160 0.02160 0.02160 0.02162

Eigenvalues --- 0.02162 0.02162 0.02162 0.02173 0.02173

Eigenvalues --- 0.02173 0.02176 0.02181 0.02181 0.02182

Eigenvalues --- 0.02184 0.02186 0.02187 0.02187 0.02190

Eigenvalues --- 0.02216 0.02217 0.02346 0.02756 0.04345

Eigenvalues --- 0.15901 0.15949 0.15950 0.15993 0.15997

Eigenvalues --- 0.15997 0.15997 0.15997 0.15998 0.15999

Eigenvalues --- 0.15999 0.15999 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16001 0.16006 0.16031 0.16197

Eigenvalues --- 0.21890 0.22000 0.22000 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22004 0.22132 0.22759

Eigenvalues --- 0.22773 0.22816 0.22848 0.23472 0.23472

Eigenvalues --- 0.23477 0.23546 0.23874 0.24583 0.24734

Eigenvalues --- 0.24854 0.24881 0.24971 0.24985 0.24997

Eigenvalues --- 0.24998 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25001 0.25009 0.25127

Eigenvalues --- 0.26128 0.28052 0.34159 0.34187 0.34206

Eigenvalues --- 0.34965 0.35408 0.35413 0.35413 0.35413

Eigenvalues --- 0.35415 0.35415 0.35416 0.35416 0.35416

Eigenvalues --- 0.35416 0.35416 0.35427 0.35506 0.35507

Eigenvalues --- 0.35508 0.35526 0.35542 0.35545 0.35547

Eigenvalues --- 0.35762 0.36056 0.36058 0.36058 0.36111

Eigenvalues --- 0.36250 0.36251 0.36251 0.36267 0.37119

Eigenvalues --- 0.37159 0.37269 0.37294 0.37704 0.39131

Eigenvalues --- 0.39745 0.40004 0.40261 0.40424 0.40464

Eigenvalues --- 0.40899 0.41782 0.41784 0.41797 0.42091

Eigenvalues --- 0.42092 0.42094 0.42117 0.42182 0.43167

Eigenvalues --- 0.43294 0.44662 0.45477 0.45559 0.45569

Eigenvalues --- 0.45579 0.45586 0.45769 0.45776 0.45863

Eigenvalues --- 0.45900 0.45930 0.45942 0.45942 0.45948

Eigenvalues --- 0.45970 0.46628 0.46660 0.46661 0.46661

Eigenvalues --- 0.47073 0.47079 0.47086 0.47600 0.48026

Eigenvalues --- 0.48191 0.48279 0.49336 0.49433 0.49975

Eigenvalues --- 0.50721 0.50811 0.55531

En-DIIS/RFO-DIIS IScMMF= 0 using points: 10 9 8 7 6

RFO step: Lambda=-4.18893921D-08.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 4.91D-05 SmlDif= 1.00D-05

RMS Error= 0.1964616764D-04 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.05281 0.00066 -0.01914 -0.02781 -0.00653

Iteration 1 RMS(Cart)= 0.00041910 RMS(Int)= 0.00000029

Iteration 2 RMS(Cart)= 0.00000011 RMS(Int)= 0.00000029

ITry= 1 IFail=0 DXMaxC= 2.10D-03 DCOld= 1.00D+10 DXMaxT= 9.59D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 9.52D-09 for atom 50.

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

(Linear) (Quad) (Total)

R1 2.72728 0.00001 0.00001 0.00002 0.00003 2.72731

R2 2.57363 -0.00002 -0.00000 -0.00004 -0.00004 2.57358

R3 2.03836 0.00000 -0.00000 0.00001 0.00001 2.03837

R4 2.61840 -0.00001 0.00000 -0.00003 -0.00003 2.61837

R5 2.61831 -0.00001 -0.00002 -0.00003 -0.00005 2.61826

R6 2.61840 -0.00001 0.00000 -0.00003 -0.00003 2.61837

R7 1.90982 0.00000 -0.00001 0.00001 0.00000 1.90983

R8 2.72728 0.00001 0.00001 0.00002 0.00003 2.72731

R9 2.61831 -0.00001 -0.00002 -0.00003 -0.00005 2.61826

R10 2.03836 0.00000 -0.00000 0.00001 0.00001 2.03837

R11 2.70311 0.00002 -0.00002 0.00005 0.00004 2.70314

R12 2.82095 -0.00003 0.00002 -0.00007 -0.00005 2.82090

R13 2.59348 -0.00002 0.00002 -0.00005 -0.00003 2.59345

R14 2.71578 -0.00000 0.00000 -0.00000 -0.00000 2.71578

R15 2.59349 -0.00003 0.00001 -0.00006 -0.00004 2.59345

R16 2.71577 0.00000 0.00000 0.00001 0.00002 2.71579

R17 2.70309 0.00003 -0.00002 0.00008 0.00006 2.70316

R18 2.60023 0.00001 -0.00000 0.00003 0.00002 2.60026

R19 2.04092 -0.00000 0.00000 -0.00001 -0.00001 2.04091

R20 2.04091 -0.00000 0.00000 -0.00000 -0.00000 2.04091

R21 2.70311 0.00002 -0.00002 0.00005 0.00004 2.70314

R22 2.82095 -0.00003 0.00002 -0.00007 -0.00005 2.82090

R23 2.71578 -0.00000 0.00000 -0.00000 -0.00000 2.71578

R24 2.59348 -0.00002 0.00002 -0.00005 -0.00003 2.59345

R25 2.60023 0.00001 -0.00000 0.00003 0.00002 2.60026

R26 2.04091 -0.00000 0.00000 -0.00000 -0.00000 2.04091

R27 2.71577 0.00000 0.00000 0.00001 0.00002 2.71579

R28 2.04092 -0.00000 0.00000 -0.00001 -0.00001 2.04091

R29 2.59349 -0.00003 0.00001 -0.00006 -0.00004 2.59345

R30 2.70309 0.00003 -0.00002 0.00008 0.00006 2.70316

R31 2.61829 0.00001 -0.00002 0.00000 -0.00001 2.61828

R32 2.82094 -0.00002 0.00002 -0.00006 -0.00004 2.82090

R33 2.72728 0.00001 0.00001 0.00002 0.00003 2.72731

R34 2.61838 -0.00001 0.00001 -0.00002 -0.00001 2.61837

R35 2.57362 -0.00001 -0.00001 -0.00003 -0.00004 2.57358

R36 2.03836 0.00000 -0.00000 0.00000 0.00000 2.03836

R37 2.72728 0.00001 0.00001 0.00002 0.00003 2.72731

R38 2.03836 0.00000 -0.00000 0.00000 0.00000 2.03836

R39 2.61838 -0.00001 0.00001 -0.00002 -0.00001 2.61837

R40 2.61829 0.00001 -0.00002 0.00000 -0.00001 2.61828

R41 1.90982 0.00000 -0.00001 0.00001 0.00000 1.90983

R42 2.82094 -0.00002 0.00002 -0.00006 -0.00004 2.82090

R43 2.64669 -0.00001 0.00000 -0.00001 -0.00001 2.64668

R44 2.64853 0.00000 -0.00001 0.00001 -0.00000 2.64853

R45 2.63420 -0.00001 -0.00000 -0.00002 -0.00002 2.63418

R46 2.04988 0.00000 0.00000 0.00000 0.00000 2.04989

R47 2.63377 0.00000 0.00000 0.00000 0.00001 2.63377

R48 2.05087 -0.00000 0.00000 -0.00000 -0.00000 2.05087

R49 2.63634 0.00000 -0.00000 0.00001 0.00000 2.63635

R50 2.05051 -0.00000 0.00000 -0.00001 -0.00000 2.05050

R51 2.63140 -0.00001 0.00000 -0.00001 -0.00000 2.63139

R52 2.05088 -0.00000 0.00000 -0.00000 -0.00000 2.05088

R53 2.04961 -0.00000 0.00000 -0.00000 0.00000 2.04962

R54 2.63377 0.00000 0.00000 0.00000 0.00001 2.63377

R55 2.63634 0.00000 -0.00000 0.00001 0.00000 2.63635

R56 2.05051 -0.00000 0.00000 -0.00001 -0.00000 2.05050

R57 2.63420 -0.00001 -0.00000 -0.00002 -0.00002 2.63418

R58 2.05087 -0.00000 0.00000 -0.00000 -0.00000 2.05087

R59 2.64669 -0.00001 0.00000 -0.00001 -0.00001 2.64668

R60 2.04988 0.00000 0.00000 0.00000 0.00000 2.04989

R61 2.64853 0.00000 -0.00001 0.00001 -0.00000 2.64853

R62 2.63140 -0.00001 0.00000 -0.00001 -0.00000 2.63139

R63 2.04961 -0.00000 0.00000 -0.00000 0.00000 2.04962

R64 2.05088 -0.00000 0.00000 -0.00000 -0.00000 2.05088

R65 2.64852 0.00001 -0.00001 0.00002 0.00001 2.64853

R66 2.64668 -0.00000 0.00000 -0.00000 0.00000 2.64669

R67 2.63140 -0.00001 0.00000 -0.00001 -0.00000 2.63139

R68 2.04961 -0.00000 0.00000 -0.00000 0.00000 2.04961

R69 2.63634 0.00000 -0.00000 0.00001 0.00000 2.63634

R70 2.05088 -0.00000 0.00000 -0.00000 -0.00000 2.05088

R71 2.63377 0.00000 0.00000 0.00000 0.00000 2.63377

R72 2.05051 -0.00000 0.00000 -0.00001 -0.00001 2.05050

R73 2.63420 -0.00001 -0.00000 -0.00001 -0.00002 2.63418

R74 2.05087 -0.00000 0.00000 -0.00000 -0.00000 2.05087

R75 2.04988 0.00000 0.00000 0.00000 0.00000 2.04989

R76 2.64852 0.00001 -0.00001 0.00002 0.00001 2.64853

R77 2.64668 -0.00000 0.00000 -0.00000 0.00000 2.64669

R78 2.63140 -0.00001 0.00000 -0.00001 -0.00000 2.63139

R79 2.04961 -0.00000 0.00000 -0.00000 0.00000 2.04961

R80 2.63634 0.00000 -0.00000 0.00001 0.00000 2.63634

R81 2.05088 -0.00000 0.00000 -0.00000 -0.00000 2.05088

R82 2.63377 0.00000 0.00000 0.00000 0.00000 2.63377

R83 2.05051 -0.00000 0.00000 -0.00001 -0.00001 2.05050

R84 2.63420 -0.00001 -0.00000 -0.00001 -0.00002 2.63418

R85 2.05087 -0.00000 0.00000 -0.00000 -0.00000 2.05087

R86 2.04988 0.00000 0.00000 0.00000 0.00000 2.04989

A1 1.89609 -0.00000 0.00000 -0.00001 -0.00001 1.89609

A2 2.17340 -0.00000 0.00000 -0.00003 -0.00003 2.17337

A3 2.21361 0.00001 -0.00001 0.00004 0.00003 2.21364

A4 1.84726 0.00001 -0.00001 0.00002 0.00001 1.84727

A5 2.21832 0.00000 0.00000 0.00001 0.00001 2.21833

A6 2.21755 -0.00001 0.00001 -0.00003 -0.00002 2.21752

A7 1.93804 -0.00001 0.00002 -0.00003 -0.00001 1.93803

A8 2.17154 0.00000 0.00002 0.00004 0.00006 2.17160

A9 2.17154 0.00000 0.00002 0.00004 0.00006 2.17160

A10 1.84726 0.00001 -0.00001 0.00002 0.00001 1.84727

A11 2.21755 -0.00001 0.00001 -0.00003 -0.00002 2.21752

A12 2.21832 0.00000 0.00000 0.00001 0.00001 2.21833

A13 1.89609 -0.00000 0.00000 -0.00001 -0.00001 1.89609

A14 2.21361 0.00001 -0.00001 0.00004 0.00003 2.21364

A15 2.17340 -0.00000 0.00000 -0.00003 -0.00003 2.17337

A16 2.19257 0.00001 0.00000 0.00002 0.00002 2.19259

A17 2.04301 0.00001 -0.00001 0.00002 0.00001 2.04302

A18 2.04761 -0.00001 0.00001 -0.00004 -0.00003 2.04758

A19 2.19206 0.00001 -0.00000 0.00003 0.00003 2.19209

A20 2.16114 -0.00001 0.00001 -0.00003 -0.00002 2.16112

A21 1.92998 -0.00000 -0.00001 -0.00000 -0.00001 1.92997

A22 1.84826 0.00002 0.00000 0.00005 0.00005 1.84831

A23 1.93000 -0.00001 -0.00000 -0.00003 -0.00003 1.92996

A24 2.19205 0.00001 -0.00000 0.00004 0.00003 2.19208

A25 2.16114 -0.00000 0.00001 -0.00001 0.00000 2.16114

A26 1.85816 -0.00000 0.00000 0.00001 0.00001 1.85817

A27 2.20396 -0.00001 0.00002 -0.00006 -0.00004 2.20392

A28 2.22098 0.00001 -0.00002 0.00005 0.00003 2.22101

A29 1.85818 -0.00001 0.00001 -0.00003 -0.00002 1.85816

A30 2.20394 -0.00001 0.00002 -0.00005 -0.00003 2.20392

A31 2.22097 0.00002 -0.00002 0.00007 0.00005 2.22102

A32 2.19257 0.00001 0.00000 0.00002 0.00002 2.19259

A33 2.04301 0.00001 -0.00001 0.00002 0.00001 2.04302

A34 2.04761 -0.00001 0.00001 -0.00004 -0.00003 2.04758

A35 2.16114 -0.00001 0.00001 -0.00003 -0.00002 2.16112

A36 2.19206 0.00001 -0.00000 0.00003 0.00003 2.19209

A37 1.92998 -0.00000 -0.00001 -0.00000 -0.00001 1.92997

A38 1.85818 -0.00001 0.00001 -0.00003 -0.00002 1.85816

A39 2.20394 -0.00001 0.00002 -0.00005 -0.00003 2.20392

A40 2.22097 0.00002 -0.00002 0.00007 0.00005 2.22102

A41 1.85816 -0.00000 0.00000 0.00001 0.00001 1.85817

A42 2.22098 0.00001 -0.00002 0.00005 0.00003 2.22101

A43 2.20396 -0.00001 0.00002 -0.00006 -0.00004 2.20392

A44 1.93000 -0.00001 -0.00000 -0.00003 -0.00003 1.92996

A45 2.16114 -0.00000 0.00001 -0.00001 0.00000 2.16114

A46 2.19205 0.00001 -0.00000 0.00004 0.00003 2.19208

A47 1.84826 0.00002 0.00000 0.00005 0.00005 1.84831

A48 2.19257 0.00000 0.00000 0.00001 0.00001 2.19258

A49 2.04761 -0.00001 0.00001 -0.00004 -0.00003 2.04758

A50 2.04300 0.00001 -0.00001 0.00003 0.00002 2.04302

A51 2.21831 0.00001 -0.00000 0.00002 0.00002 2.21833

A52 2.21755 -0.00001 0.00001 -0.00003 -0.00001 2.21753

A53 1.84726 0.00000 -0.00001 0.00000 -0.00001 1.84725

A54 1.89609 -0.00000 0.00001 -0.00000 0.00000 1.89609

A55 2.17339 -0.00000 0.00001 -0.00003 -0.00002 2.17337

A56 2.21362 0.00001 -0.00001 0.00003 0.00002 2.21364

A57 1.89609 -0.00000 0.00001 -0.00000 0.00000 1.89609

A58 2.21362 0.00001 -0.00001 0.00003 0.00002 2.21364

A59 2.17339 -0.00000 0.00001 -0.00003 -0.00002 2.17337

A60 1.84726 0.00000 -0.00001 0.00000 -0.00001 1.84725

A61 2.21831 0.00001 -0.00000 0.00002 0.00002 2.21833

A62 2.21755 -0.00001 0.00001 -0.00003 -0.00001 2.21753

A63 1.93803 0.00000 0.00001 -0.00000 0.00001 1.93804

A64 2.17158 -0.00000 0.00001 0.00002 0.00003 2.17161

A65 2.17158 -0.00000 0.00001 0.00002 0.00003 2.17161

A66 2.19257 0.00000 0.00000 0.00001 0.00001 2.19258

A67 2.04761 -0.00001 0.00001 -0.00004 -0.00003 2.04758

A68 2.04300 0.00001 -0.00001 0.00003 0.00002 2.04302

A69 2.11281 0.00001 -0.00003 0.00003 0.00001 2.11281

A70 2.10399 -0.00002 0.00003 -0.00005 -0.00002 2.10397

A71 2.06638 0.00001 -0.00000 0.00002 0.00002 2.06640

A72 2.10932 -0.00000 0.00001 -0.00001 -0.00001 2.10931

A73 2.08175 0.00000 -0.00001 0.00002 0.00001 2.08176

A74 2.09210 -0.00000 0.00000 -0.00000 -0.00000 2.09210

A75 2.09737 0.00000 -0.00000 0.00001 0.00000 2.09737

A76 2.08926 -0.00000 0.00001 -0.00002 -0.00002 2.08924

A77 2.09655 0.00000 -0.00000 0.00002 0.00002 2.09656

A78 2.08634 0.00000 -0.00000 0.00000 0.00000 2.08635

A79 2.09862 -0.00000 0.00000 -0.00001 -0.00001 2.09862

A80 2.09822 0.00000 -0.00000 0.00001 0.00000 2.09822

A81 2.09751 -0.00000 0.00000 -0.00000 -0.00000 2.09751

A82 2.09603 0.00000 -0.00000 0.00003 0.00002 2.09605

A83 2.08964 -0.00000 0.00000 -0.00003 -0.00002 2.08961

A84 2.10942 -0.00001 0.00000 -0.00002 -0.00001 2.10941

A85 2.08152 0.00001 -0.00000 0.00003 0.00003 2.08155

A86 2.09222 -0.00000 0.00000 -0.00002 -0.00002 2.09220

A87 2.08634 0.00000 -0.00000 0.00000 0.00000 2.08635

A88 2.09862 -0.00000 0.00000 -0.00001 -0.00001 2.09862

A89 2.09822 0.00000 -0.00000 0.00001 0.00000 2.09822

A90 2.09737 0.00000 -0.00000 0.00001 0.00000 2.09737

A91 2.09655 0.00000 -0.00000 0.00002 0.00002 2.09656

A92 2.08926 -0.00000 0.00001 -0.00002 -0.00002 2.08924

A93 2.10932 -0.00000 0.00001 -0.00001 -0.00001 2.10931

A94 2.09210 -0.00000 0.00000 -0.00000 -0.00000 2.09210

A95 2.08175 0.00000 -0.00001 0.00002 0.00001 2.08176

A96 2.11281 0.00001 -0.00003 0.00003 0.00001 2.11281

A97 2.10399 -0.00002 0.00003 -0.00005 -0.00002 2.10397

A98 2.06638 0.00001 -0.00000 0.00002 0.00002 2.06640

A99 2.10942 -0.00001 0.00000 -0.00002 -0.00001 2.10941

A100 2.08152 0.00001 -0.00000 0.00003 0.00003 2.08155

A101 2.09222 -0.00000 0.00000 -0.00002 -0.00002 2.09220

A102 2.09751 -0.00000 0.00000 -0.00000 -0.00000 2.09751

A103 2.09603 0.00000 -0.00000 0.00003 0.00002 2.09605

A104 2.08964 -0.00000 0.00000 -0.00003 -0.00002 2.08961

A105 2.10401 -0.00002 0.00003 -0.00006 -0.00003 2.10398

A106 2.11278 0.00001 -0.00003 0.00005 0.00003 2.11281

A107 2.06639 0.00000 -0.00001 0.00001 0.00000 2.06639

A108 2.10941 -0.00000 0.00000 -0.00001 -0.00000 2.10941

A109 2.08152 0.00001 -0.00000 0.00003 0.00003 2.08155

A110 2.09222 -0.00000 0.00000 -0.00002 -0.00002 2.09220

A111 2.09751 -0.00000 0.00000 0.00000 0.00000 2.09752

A112 2.08964 -0.00000 0.00000 -0.00003 -0.00003 2.08961

A113 2.09603 0.00000 -0.00000 0.00003 0.00003 2.09605

A114 2.08635 0.00000 -0.00000 -0.00000 -0.00000 2.08634

A115 2.09822 0.00000 -0.00000 0.00001 0.00001 2.09822

A116 2.09862 -0.00000 0.00000 -0.00000 -0.00000 2.09862

A117 2.09737 0.00000 -0.00000 0.00001 0.00000 2.09737

A118 2.09655 0.00000 -0.00000 0.00002 0.00002 2.09656

A119 2.08926 -0.00000 0.00001 -0.00003 -0.00002 2.08924

A120 2.10931 -0.00000 0.00001 -0.00001 0.00000 2.10931

A121 2.08175 0.00000 -0.00001 0.00001 0.00001 2.08176

A122 2.09210 -0.00000 -0.00000 -0.00001 -0.00001 2.09210

A123 2.10401 -0.00002 0.00003 -0.00006 -0.00003 2.10398

A124 2.11278 0.00001 -0.00003 0.00005 0.00003 2.11281

A125 2.06639 0.00000 -0.00001 0.00001 0.00000 2.06639

A126 2.10941 -0.00000 0.00000 -0.00001 -0.00000 2.10941

A127 2.08152 0.00001 -0.00000 0.00003 0.00003 2.08155

A128 2.09222 -0.00000 0.00000 -0.00002 -0.00002 2.09220

A129 2.09751 -0.00000 0.00000 0.00000 0.00000 2.09752

A130 2.08964 -0.00000 0.00000 -0.00003 -0.00003 2.08961

A131 2.09603 0.00000 -0.00000 0.00003 0.00003 2.09605

A132 2.08635 0.00000 -0.00000 -0.00000 -0.00000 2.08634

A133 2.09822 0.00000 -0.00000 0.00001 0.00001 2.09822

A134 2.09862 -0.00000 0.00000 -0.00000 -0.00000 2.09862

A135 2.09737 0.00000 -0.00000 0.00001 0.00000 2.09737

A136 2.09655 0.00000 -0.00000 0.00002 0.00002 2.09656

A137 2.08926 -0.00000 0.00001 -0.00003 -0.00002 2.08924

A138 2.10931 -0.00000 0.00001 -0.00001 0.00000 2.10931

A139 2.08175 0.00000 -0.00001 0.00001 0.00001 2.08176

A140 2.09210 -0.00000 -0.00000 -0.00001 -0.00001 2.09210

D1 0.00505 0.00000 0.00008 0.00026 0.00035 0.00540

D2 3.13524 -0.00000 0.00012 0.00004 0.00016 3.13540

D3 -3.12321 0.00000 0.00015 0.00016 0.00031 -3.12290

D4 0.00697 -0.00000 0.00018 -0.00006 0.00012 0.00710

D5 -0.00000 0.00000 -0.00000 -0.00000 0.00000 0.00000

D6 -3.12788 -0.00000 0.00006 -0.00010 -0.00004 -3.12791

D7 3.12788 0.00000 -0.00006 0.00010 0.00004 3.12791

D8 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D9 -0.00846 -0.00001 -0.00014 -0.00044 -0.00058 -0.00904

D10 3.06671 0.00001 0.00063 0.00050 0.00113 3.06784

D11 -3.13865 -0.00000 -0.00018 -0.00022 -0.00039 -3.13904

D12 -0.06348 0.00001 0.00059 0.00073 0.00132 -0.06217

D13 -3.08319 -0.00000 -0.00011 -0.00017 -0.00027 -3.08347

D14 0.05624 -0.00000 -0.00010 -0.00002 -0.00012 0.05612

D15 0.04465 -0.00001 -0.00006 -0.00043 -0.00050 0.04415

D16 -3.09910 -0.00001 -0.00006 -0.00029 -0.00035 -3.09945

D17 0.00846 0.00001 0.00014 0.00044 0.00058 0.00904

D18 3.13865 0.00000 0.00018 0.00022 0.00039 3.13904

D19 -3.06671 -0.00001 -0.00063 -0.00050 -0.00113 -3.06784

D20 0.06348 -0.00001 -0.00059 -0.00073 -0.00132 0.06217

D21 -0.00505 -0.00000 -0.00008 -0.00026 -0.00035 -0.00540

D22 3.12321 -0.00000 -0.00015 -0.00016 -0.00031 3.12290

D23 -3.13524 0.00000 -0.00012 -0.00004 -0.00016 -3.13540

D24 -0.00697 0.00000 -0.00018 0.00006 -0.00012 -0.00710

D25 -0.04465 0.00001 0.00006 0.00043 0.00050 -0.04415

D26 3.09910 0.00001 0.00006 0.00029 0.00035 3.09945

D27 3.08319 0.00000 0.00011 0.00017 0.00027 3.08347

D28 -0.05624 0.00000 0.00010 0.00002 0.00012 -0.05612

D29 -0.10884 -0.00000 0.00021 -0.00003 0.00017 -0.10866

D30 3.02964 -0.00000 0.00018 -0.00007 0.00012 3.02976

D31 3.03060 0.00000 0.00021 0.00011 0.00033 3.03092

D32 -0.11411 0.00000 0.00019 0.00008 0.00027 -0.11384

D33 -1.12673 0.00000 -0.00017 0.00030 0.00013 -1.12661

D34 2.01623 0.00000 -0.00017 0.00042 0.00025 2.01648

D35 2.01683 0.00000 -0.00018 0.00016 -0.00001 2.01682

D36 -1.12339 0.00000 -0.00018 0.00029 0.00011 -1.12328

D37 -3.12576 -0.00000 -0.00002 -0.00002 -0.00004 -3.12580

D38 0.01859 -0.00000 -0.00001 0.00002 0.00001 0.01861

D39 3.13265 -0.00000 0.00002 -0.00006 -0.00003 3.13262

D40 -0.02256 0.00000 0.00002 0.00011 0.00013 -0.02243

D41 -0.01164 -0.00000 0.00001 -0.00009 -0.00008 -0.01173

D42 3.11633 0.00000 0.00000 0.00007 0.00008 3.11641

D43 -0.01863 0.00000 0.00000 0.00006 0.00006 -0.01857

D44 3.12574 0.00000 0.00002 0.00002 0.00004 3.12579

D45 0.01174 -0.00000 0.00000 -0.00011 -0.00011 0.01163

D46 -3.11630 -0.00000 -0.00000 -0.00013 -0.00013 -3.11643

D47 -3.13257 -0.00000 -0.00002 -0.00008 -0.00010 -3.13267

D48 0.02257 -0.00000 -0.00002 -0.00009 -0.00011 0.02246

D49 0.10870 0.00000 -0.00021 0.00014 -0.00007 0.10863

D50 -3.03081 0.00000 -0.00022 0.00012 -0.00010 -3.03091

D51 -3.02975 0.00000 -0.00018 0.00009 -0.00009 -3.02984

D52 0.11392 0.00000 -0.00019 0.00008 -0.00012 0.11380

D53 -0.00006 0.00000 -0.00000 0.00012 0.00011 0.00006

D54 -3.12786 -0.00000 -0.00000 -0.00005 -0.00005 -3.12791

D55 3.12781 0.00000 -0.00000 0.00013 0.00013 3.12794

D56 0.00001 -0.00000 0.00000 -0.00003 -0.00003 -0.00002

D57 -3.02964 0.00000 -0.00018 0.00007 -0.00012 -3.02976

D58 0.10884 0.00000 -0.00021 0.00003 -0.00017 0.10866

D59 0.11411 -0.00000 -0.00019 -0.00008 -0.00027 0.11384

D60 -3.03060 -0.00000 -0.00021 -0.00011 -0.00033 -3.03092

D61 1.12673 -0.00000 0.00017 -0.00030 -0.00013 1.12661

D62 -2.01623 -0.00000 0.00017 -0.00042 -0.00025 -2.01648

D63 -2.01683 -0.00000 0.00018 -0.00016 0.00001 -2.01682

D64 1.12339 -0.00000 0.00018 -0.00029 -0.00011 1.12328

D65 -3.13265 0.00000 -0.00002 0.00006 0.00003 -3.13262

D66 0.02256 -0.00000 -0.00002 -0.00011 -0.00013 0.02243

D67 0.01164 0.00000 -0.00001 0.00009 0.00008 0.01173

D68 -3.11633 -0.00000 -0.00000 -0.00007 -0.00008 -3.11641

D69 3.12576 0.00000 0.00002 0.00002 0.00004 3.12580

D70 -0.01859 0.00000 0.00001 -0.00002 -0.00001 -0.01861

D71 0.00006 -0.00000 0.00000 -0.00012 -0.00011 -0.00006

D72 -3.12781 -0.00000 0.00000 -0.00013 -0.00013 -3.12794

D73 3.12786 0.00000 0.00000 0.00005 0.00005 3.12791

D74 -0.00001 0.00000 -0.00000 0.00003 0.00003 0.00002

D75 -0.01174 0.00000 -0.00000 0.00011 0.00011 -0.01163

D76 3.13257 0.00000 0.00002 0.00008 0.00010 3.13267

D77 3.11630 0.00000 0.00000 0.00013 0.00013 3.11643

D78 -0.02257 0.00000 0.00002 0.00009 0.00011 -0.02246

D79 0.01863 -0.00000 -0.00000 -0.00006 -0.00006 0.01857

D80 -3.12574 -0.00000 -0.00002 -0.00002 -0.00004 -3.12579

D81 3.02975 -0.00000 0.00018 -0.00009 0.00009 3.02984

D82 -0.11392 -0.00000 0.00019 -0.00008 0.00012 -0.11380

D83 -0.10870 -0.00000 0.00021 -0.00014 0.00007 -0.10863

D84 3.03081 -0.00000 0.00022 -0.00012 0.00010 3.03091

D85 3.08328 -0.00000 0.00011 -0.00001 0.00009 3.08337

D86 -0.04461 0.00001 0.00005 0.00037 0.00042 -0.04420

D87 -0.05624 -0.00000 0.00010 -0.00003 0.00007 -0.05617

D88 3.09905 0.00001 0.00003 0.00036 0.00039 3.09944

D89 -1.12324 0.00000 -0.00014 0.00001 -0.00014 -1.12338

D90 2.01697 -0.00000 -0.00015 -0.00011 -0.00025 2.01672

D91 2.01645 -0.00000 -0.00013 0.00002 -0.00011 2.01634

D92 -1.12652 -0.00000 -0.00014 -0.00009 -0.00023 -1.12675

D93 -3.13542 0.00000 -0.00012 0.00013 0.00001 -3.13541

D94 -0.00718 0.00000 -0.00018 0.00018 0.00000 -0.00718

D95 -0.00519 -0.00000 -0.00007 -0.00019 -0.00026 -0.00545

D96 3.12305 -0.00000 -0.00012 -0.00014 -0.00027 3.12278

D97 3.13892 -0.00000 0.00017 -0.00000 0.00017 3.13908

D98 0.06276 -0.00001 -0.00041 -0.00059 -0.00100 0.06176

D99 0.00868 0.00001 0.00012 0.00032 0.00043 0.00912

D100 -3.06748 -0.00000 -0.00047 -0.00026 -0.00073 -3.06821

D101 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D102 3.12784 0.00000 -0.00006 0.00005 -0.00001 3.12783

D103 -3.12784 -0.00000 0.00006 -0.00005 0.00001 -3.12783

D104 -0.00000 -0.00000 -0.00000 -0.00000 0.00000 0.00000

D105 0.00519 0.00000 0.00007 0.00019 0.00026 0.00545

D106 3.13542 -0.00000 0.00012 -0.00013 -0.00001 3.13541

D107 -3.12305 0.00000 0.00012 0.00014 0.00027 -3.12278

D108 0.00718 -0.00000 0.00018 -0.00018 -0.00000 0.00718

D109 -0.00868 -0.00001 -0.00012 -0.00032 -0.00043 -0.00912

D110 3.06748 0.00000 0.00047 0.00026 0.00073 3.06821

D111 -3.13892 0.00000 -0.00017 0.00000 -0.00017 -3.13908

D112 -0.06276 0.00001 0.00041 0.00059 0.00100 -0.06176

D113 -3.08328 0.00000 -0.00011 0.00001 -0.00009 -3.08337

D114 0.05624 0.00000 -0.00010 0.00003 -0.00007 0.05617

D115 0.04461 -0.00001 -0.00005 -0.00037 -0.00042 0.04420

D116 -3.09905 -0.00001 -0.00003 -0.00036 -0.00039 -3.09944

D117 1.12324 -0.00000 0.00014 -0.00001 0.00014 1.12338

D118 -2.01697 0.00000 0.00015 0.00011 0.00025 -2.01672

D119 -2.01645 0.00000 0.00013 -0.00002 0.00011 -2.01634

D120 1.12652 0.00000 0.00014 0.00009 0.00023 1.12675

D121 3.13729 0.00000 0.00000 0.00018 0.00018 3.13747

D122 -0.01075 0.00000 0.00002 0.00007 0.00009 -0.01067

D123 -0.00564 0.00000 -0.00000 0.00005 0.00005 -0.00559

D124 3.12950 -0.00000 0.00001 -0.00005 -0.00004 3.12946

D125 -3.13622 -0.00000 -0.00001 -0.00012 -0.00014 -3.13635

D126 -0.00299 -0.00000 -0.00000 -0.00009 -0.00010 -0.00308

D127 0.00671 0.00000 -0.00001 -0.00000 -0.00001 0.00670

D128 3.13994 0.00000 -0.00000 0.00003 0.00003 3.13997

D129 0.00188 -0.00000 0.00001 -0.00008 -0.00007 0.00181

D130 3.13868 -0.00000 0.00002 -0.00005 -0.00003 3.13864

D131 -3.13323 0.00000 -0.00001 0.00003 0.00002 -3.13321

D132 0.00358 0.00000 0.00000 0.00006 0.00006 0.00363

D133 0.00097 0.00000 -0.00001 0.00005 0.00005 0.00101

D134 -3.14143 0.00000 -0.00001 0.00004 0.00004 -3.14140

D135 -3.13582 0.00000 -0.00001 0.00002 0.00001 -3.13581

D136 0.00497 0.00000 -0.00001 0.00002 0.00000 0.00497

D137 0.00009 0.00000 -0.00001 -0.00000 -0.00001 0.00008

D138 -3.13737 -0.00000 -0.00001 -0.00001 -0.00002 -3.13739

D139 -3.14069 0.00000 -0.00000 0.00001 0.00000 -3.14069

D140 0.00503 -0.00000 -0.00001 -0.00000 -0.00001 0.00502

D141 -0.00401 -0.00000 0.00001 -0.00002 -0.00001 -0.00402

D142 -3.13719 -0.00000 0.00001 -0.00006 -0.00005 -3.13724

D143 3.13346 -0.00000 0.00002 -0.00001 0.00000 3.13346

D144 0.00028 -0.00000 0.00001 -0.00005 -0.00004 0.00025

D145 -0.00097 -0.00000 0.00001 -0.00005 -0.00005 -0.00101

D146 3.13582 -0.00000 0.00001 -0.00002 -0.00001 3.13581

D147 3.14143 -0.00000 0.00001 -0.00004 -0.00004 3.14140

D148 -0.00497 -0.00000 0.00001 -0.00002 -0.00000 -0.00497

D149 -0.00009 -0.00000 0.00001 0.00000 0.00001 -0.00008

D150 3.13737 0.00000 0.00001 0.00001 0.00002 3.13739

D151 3.14069 -0.00000 0.00000 -0.00001 -0.00000 3.14069

D152 -0.00503 0.00000 0.00001 0.00000 0.00001 -0.00502

D153 -0.00188 0.00000 -0.00001 0.00008 0.00007 -0.00181

D154 3.13323 -0.00000 0.00001 -0.00003 -0.00002 3.13321

D155 -3.13868 0.00000 -0.00002 0.00005 0.00003 -3.13864

D156 -0.00358 -0.00000 -0.00000 -0.00006 -0.00006 -0.00363

D157 -3.13729 -0.00000 -0.00000 -0.00018 -0.00018 -3.13747

D158 0.00564 -0.00000 0.00000 -0.00005 -0.00005 0.00559

D159 0.01075 -0.00000 -0.00002 -0.00007 -0.00009 0.01067

D160 -3.12950 0.00000 -0.00001 0.00005 0.00004 -3.12946

D161 3.13622 0.00000 0.00001 0.00012 0.00014 3.13635

D162 0.00299 0.00000 0.00000 0.00009 0.00010 0.00308

D163 -0.00671 -0.00000 0.00001 0.00000 0.00001 -0.00670

D164 -3.13994 -0.00000 0.00000 -0.00003 -0.00003 -3.13997

D165 0.00401 0.00000 -0.00001 0.00002 0.00001 0.00402

D166 -3.13346 0.00000 -0.00002 0.00001 -0.00000 -3.13346

D167 3.13719 0.00000 -0.00001 0.00006 0.00005 3.13724

D168 -0.00028 0.00000 -0.00001 0.00005 0.00004 -0.00025

D169 3.13625 0.00000 0.00002 0.00009 0.00011 3.13635

D170 0.00300 0.00000 0.00001 0.00010 0.00011 0.00311

D171 -0.00669 -0.00000 0.00001 -0.00002 -0.00001 -0.00670

D172 -3.13994 -0.00000 0.00000 -0.00001 -0.00001 -3.13995

D173 -3.13730 -0.00000 -0.00000 -0.00017 -0.00018 -3.13748

D174 0.01072 -0.00000 -0.00001 -0.00003 -0.00004 0.01068

D175 0.00564 -0.00000 0.00000 -0.00006 -0.00006 0.00558

D176 -3.12952 0.00000 -0.00001 0.00008 0.00008 -3.12944

D177 0.00399 0.00000 -0.00002 0.00006 0.00004 0.00403

D178 -3.13348 0.00000 -0.00002 0.00004 0.00003 -3.13346

D179 3.13718 0.00000 -0.00001 0.00005 0.00004 3.13722

D180 -0.00029 0.00000 -0.00001 0.00004 0.00003 -0.00026

D181 -0.00008 -0.00000 0.00001 -0.00001 -0.00001 -0.00009

D182 3.14071 -0.00000 0.00000 -0.00003 -0.00002 3.14068

D183 3.13737 0.00000 0.00001 0.00000 0.00001 3.13738

D184 -0.00502 -0.00000 0.00001 -0.00002 -0.00001 -0.00503

D185 -0.00095 -0.00000 0.00001 -0.00007 -0.00006 -0.00102

D186 3.13584 -0.00000 0.00001 -0.00005 -0.00004 3.13580

D187 3.14144 -0.00000 0.00001 -0.00005 -0.00005 3.14139

D188 -0.00495 -0.00000 0.00001 -0.00003 -0.00002 -0.00497

D189 -0.00189 0.00000 -0.00001 0.00011 0.00010 -0.00179

D190 3.13323 -0.00000 -0.00000 -0.00004 -0.00004 3.13319

D191 -3.13871 0.00000 -0.00002 0.00009 0.00007 -3.13864

D192 -0.00358 -0.00000 -0.00001 -0.00006 -0.00007 -0.00365

D193 -3.13625 -0.00000 -0.00002 -0.00009 -0.00011 -3.13635

D194 -0.00300 -0.00000 -0.00001 -0.00010 -0.00011 -0.00311

D195 0.00669 0.00000 -0.00001 0.00002 0.00001 0.00670

D196 3.13994 0.00000 -0.00000 0.00001 0.00001 3.13995

D197 3.13730 0.00000 0.00000 0.00017 0.00018 3.13748

D198 -0.01072 0.00000 0.00001 0.00003 0.00004 -0.01068

D199 -0.00564 0.00000 -0.00000 0.00006 0.00006 -0.00558

D200 3.12952 -0.00000 0.00001 -0.00008 -0.00008 3.12944

D201 -0.00399 -0.00000 0.00002 -0.00006 -0.00004 -0.00403

D202 3.13348 -0.00000 0.00002 -0.00004 -0.00003 3.13346

D203 -3.13718 -0.00000 0.00001 -0.00005 -0.00004 -3.13722

D204 0.00029 -0.00000 0.00001 -0.00004 -0.00003 0.00026

D205 0.00008 0.00000 -0.00001 0.00001 0.00001 0.00009

D206 -3.14071 0.00000 -0.00000 0.00003 0.00002 -3.14068

D207 -3.13737 -0.00000 -0.00001 -0.00000 -0.00001 -3.13738

D208 0.00502 0.00000 -0.00001 0.00002 0.00001 0.00503

D209 0.00095 0.00000 -0.00001 0.00007 0.00006 0.00102

D210 -3.13584 0.00000 -0.00001 0.00005 0.00004 -3.13580

D211 -3.14144 0.00000 -0.00001 0.00005 0.00005 -3.14139

D212 0.00495 0.00000 -0.00001 0.00003 0.00002 0.00497

D213 0.00189 -0.00000 0.00001 -0.00011 -0.00010 0.00179

D214 -3.13323 0.00000 0.00000 0.00004 0.00004 -3.13319

D215 3.13871 -0.00000 0.00002 -0.00009 -0.00007 3.13864

D216 0.00358 0.00000 0.00001 0.00006 0.00007 0.00365

Item Value Threshold Converged?

Maximum Force 0.000033 0.000450 YES

RMS Force 0.000007 0.000300 YES

Maximum Displacement 0.002101 0.001800 NO

RMS Displacement 0.000419 0.001200 YES

Predicted change in Energy=-8.503887D-08

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Aug 18 15:03:20 2019, MaxMem= 2013265920 cpu: 1.4

(Enter /home/kira/g09/l202.exe)

Stoichiometry C44H30N4(1-,2)

Framework group CS[SG(H2N2),X(C44H28N2)]

Deg. of freedom 116

Full point group CS NOp 2

RotChk: IX=3 Diff= 8.40D-06

Largest Abelian subgroup CS NOp 2

Largest concise Abelian subgroup CS NOp 2

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 4.259425 -0.136212 0.680941

2 6 0 2.898045 -0.006510 1.142174

3 7 0 2.116534 0.060719 -0.000000

4 6 0 2.898045 -0.006510 -1.142174

5 6 0 4.259425 -0.136212 -0.680941

6 6 0 2.460576 0.028292 -2.456362

7 6 0 1.095329 0.090736 -2.878694

8 7 0 -0.000001 0.005126 -2.056266

9 6 0 -1.095320 0.090756 -2.878707

10 6 0 -0.687976 0.258285 -4.246682

11 6 0 0.688020 0.258320 -4.246668

12 6 0 2.460576 0.028292 2.456362

13 6 0 1.095329 0.090736 2.878694

14 6 0 0.688020 0.258320 4.246668

15 6 0 -0.687976 0.258285 4.246682

16 6 0 -1.095320 0.090756 2.878707

17 7 0 -0.000001 0.005126 2.056266

18 6 0 -2.460574 0.028318 2.456376

19 6 0 -2.898039 -0.006527 1.142180

20 6 0 -4.259409 -0.136332 0.680940

21 6 0 -4.259409 -0.136332 -0.680940

22 6 0 -2.898039 -0.006527 -1.142180

23 7 0 -2.116538 0.060696 0.000000

24 6 0 -2.460574 0.028318 -2.456376

25 6 0 3.506228 -0.004777 -3.521177

26 6 0 4.426960 1.041117 -3.662366

27 6 0 5.404782 1.003624 -4.655113

28 6 0 5.477023 -0.081710 -5.526504

29 6 0 4.563641 -1.128447 -5.398586

30 6 0 3.586981 -1.087975 -4.406883

31 6 0 5.477023 -0.081710 5.526504

32 6 0 5.404782 1.003624 4.655113

33 6 0 4.426960 1.041117 3.662366

34 6 0 3.506228 -0.004777 3.521177

35 6 0 3.586981 -1.087975 4.406883

36 6 0 4.563641 -1.128447 5.398586

37 6 0 -3.506229 -0.004755 -3.521190

38 6 0 -3.587078 -1.088005 -4.406825

39 6 0 -4.563750 -1.128466 -5.398519

40 6 0 -5.477043 -0.081661 -5.526509

41 6 0 -5.404706 1.003728 -4.655194

42 6 0 -4.426882 1.041204 -3.662449

43 6 0 -3.506229 -0.004755 3.521190

44 6 0 -3.587078 -1.088005 4.406825

45 6 0 -4.563750 -1.128466 5.398519

46 6 0 -5.477043 -0.081661 5.526509

47 6 0 -5.404706 1.003728 4.655194

48 6 0 -4.426882 1.041204 3.662449

49 1 0 5.117681 -0.229845 1.327571

50 1 0 5.117681 -0.229845 -1.327571

51 1 0 -1.341754 0.374441 -5.098436

52 1 0 1.341822 0.374492 -5.098404

53 1 0 1.341822 0.374492 5.098404

54 1 0 -1.341754 0.374441 5.098436

55 1 0 -5.117653 -0.230096 1.327566

56 1 0 -5.117653 -0.230096 -1.327566

57 1 0 4.370285 1.891877 -2.991779

58 1 0 6.107124 1.825591 -4.749491

59 1 0 6.237826 -0.112174 -6.299581

60 1 0 4.614106 -1.979810 -6.069753

61 1 0 2.881914 -1.906348 -4.309290

62 1 0 6.237826 -0.112174 6.299581

63 1 0 6.107124 1.825591 4.749491

64 1 0 4.370285 1.891877 2.991779

65 1 0 2.881914 -1.906348 4.309290

66 1 0 4.614106 -1.979810 6.069753

67 1 0 -2.882093 -1.906439 -4.309171

68 1 0 -4.614292 -1.979873 -6.069623

69 1 0 -6.237849 -0.112114 -6.299584

70 1 0 -6.106977 1.825750 -4.749629

71 1 0 -4.370127 1.892012 -2.991933

72 1 0 -2.882093 -1.906439 4.309171

73 1 0 -4.614292 -1.979873 6.069623

74 1 0 -6.237849 -0.112114 6.299584

75 1 0 -6.106977 1.825750 4.749629

76 1 0 -4.370127 1.892012 2.991933

77 1 0 1.106428 0.093501 -0.000000

78 1 0 -1.106445 0.093846 0.000000

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

Rotational constants (GHZ): 0.0583459 0.0578412 0.0300209

Leave Link 202 at Sun Aug 18 15:03:20 2019, MaxMem= 2013265920 cpu: 0.1

(Enter /home/kira/g09/l301.exe)

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

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

There are 513 symmetry adapted cartesian basis functions of A' symmetry.

There are 489 symmetry adapted cartesian basis functions of A" symmetry.

There are 488 symmetry adapted basis functions of A' symmetry.

There are 466 symmetry adapted basis functions of A" symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 161 beta electrons

nuclear repulsion energy 5346.0809742312 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= 78 NActive= 78 NUniq= 41 SFac= 3.62D+00 NAtFMM= 60 NAOKFM=T 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= -0.2116697781 Hartrees.

Nuclear repulsion after empirical dispersion term = 5345.8693044531 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= 78.

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

Smoothing algorithm: York/Karplus (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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5706

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.12D-08

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 282

GePol: Fraction of low-weight points (<1% of avg) = 4.94%

GePol: Cavity surface area = 617.903 Ang\*\*2

GePol: Cavity volume = 629.233 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0019878043 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5345.8673166489 Hartrees.

Leave Link 301 at Sun Aug 18 15:03:20 2019, MaxMem= 2013265920 cpu: 1.1

(Enter /home/kira/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.

One-electron integral symmetry used in STVInt

NBasis= 954 RedAO= T EigKep= 8.98D-05 NBF= 488 466

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 488 466

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= 938 938 939 939 940 MxSgAt= 78 MxSgA2= 78.

Leave Link 302 at Sun Aug 18 15:03:21 2019, MaxMem= 2013265920 cpu: 10.2

(Enter /home/kira/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sun Aug 18 15:03:22 2019, MaxMem= 2013265920 cpu: 1.2

(Enter /home/kira/g09/l401.exe)

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

B after Tr= 0.000000 -0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000004 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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The electronic state of the initial guess is 2-A'.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7586 S= 0.5043

Leave Link 401 at Sun Aug 18 15:03:26 2019, MaxMem= 2013265920 cpu: 33.5

(Enter /home/kira/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3047318 IEndB= 3047318 NGot= 2013265920 MDV= 2011240249

LenX= 2011240249 LenY= 2010235243

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= 480000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 97675308.

Iteration 1 A\*A^-1 deviation from unit magnitude is 9.99D-15 for 5705.

Iteration 1 A\*A^-1 deviation from orthogonality is 7.44D-15 for 5705 51.

Iteration 1 A^-1\*A deviation from unit magnitude is 1.02D-14 for 5705.

Iteration 1 A^-1\*A deviation from orthogonality is 2.87D-09 for 4418 4391.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.44D-15 for 2665.

Iteration 2 A\*A^-1 deviation from orthogonality is 3.11D-15 for 4904 750.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 3605.

Iteration 2 A^-1\*A deviation from orthogonality is 4.44D-16 for 5215 3288.

E= -1914.49362682841

DIIS: error= 2.89D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.49362682841 IErMin= 1 ErrMin= 2.89D-05

ErrMax= 2.89D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.69D-06 BMatP= 2.69D-06

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

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 0.446 Goal= None Shift= 0.000

Gap= 0.504 Goal= None Shift= 0.000

RMSDP=1.46D-06 MaxDP=5.09D-05 OVMax= 1.51D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.46D-06 CP: 1.00D+00

E= -1914.49362805630 Delta-E= -0.000001227892 Rises=F Damp=F

DIIS: error= 3.24D-06 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.49362805630 IErMin= 2 ErrMin= 3.24D-06

ErrMax= 3.24D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.97D-08 BMatP= 2.69D-06

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

Coeff-Com: -0.666D-01 0.107D+01

Coeff: -0.666D-01 0.107D+01

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=2.00D-07 MaxDP=1.10D-05 DE=-1.23D-06 OVMax= 2.06D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.72D-07 CP: 1.00D+00 1.07D+00

E= -1914.49362807134 Delta-E= -0.000000015039 Rises=F Damp=F

DIIS: error= 1.53D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.49362807134 IErMin= 3 ErrMin= 1.53D-06

ErrMax= 1.53D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.05D-08 BMatP= 2.97D-08

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

Coeff-Com: -0.315D-01 0.432D+00 0.599D+00

Coeff: -0.315D-01 0.432D+00 0.599D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=8.65D-08 MaxDP=4.94D-06 DE=-1.50D-08 OVMax= 1.80D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 7.93D-08 CP: 1.00D+00 1.07D+00 8.06D-01

E= -1914.49362807293 Delta-E= -0.000000001590 Rises=F Damp=F

DIIS: error= 1.35D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.49362807293 IErMin= 4 ErrMin= 1.35D-06

ErrMax= 1.35D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.07D-09 BMatP= 1.05D-08

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

Coeff-Com: -0.769D-02 0.831D-01 0.381D+00 0.543D+00

Coeff: -0.769D-02 0.831D-01 0.381D+00 0.543D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=4.46D-08 MaxDP=2.63D-06 DE=-1.59D-09 OVMax= 9.39D-06

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.39D-08 CP: 1.00D+00 1.08D+00 8.79D-01 5.64D-01

E= -1914.49362807386 Delta-E= -0.000000000938 Rises=F Damp=F

DIIS: error= 3.01D-07 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.49362807386 IErMin= 5 ErrMin= 3.01D-07

ErrMax= 3.01D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.44D-10 BMatP= 4.07D-09

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

Coeff-Com: -0.362D-03-0.633D-02 0.982D-01 0.221D+00 0.687D+00

Coeff: -0.362D-03-0.633D-02 0.982D-01 0.221D+00 0.687D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=1.27D-08 MaxDP=7.59D-07 DE=-9.38D-10 OVMax= 2.63D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 7.43D-09 CP: 1.00D+00 1.08D+00 8.94D-01 6.50D-01 7.02D-01

E= -1914.49362807398 Delta-E= -0.000000000119 Rises=F Damp=F

DIIS: error= 1.78D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.49362807398 IErMin= 6 ErrMin= 1.78D-07

ErrMax= 1.78D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.39D-11 BMatP= 1.44D-10

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

Coeff-Com: 0.735D-03-0.150D-01 0.164D-01 0.776D-01 0.451D+00 0.469D+00

Coeff: 0.735D-03-0.150D-01 0.164D-01 0.776D-01 0.451D+00 0.469D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.095 Goal= None Shift= 0.000

RMSDP=4.99D-09 MaxDP=2.96D-07 DE=-1.19D-10 OVMax= 9.98D-07

Error on total polarization charges = 0.08609

SCF Done: E(UB3LYP) = -1914.49362807 A.U. after 6 cycles

NFock= 6 Conv=0.50D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7586 S= 0.5043

<L.S>= 0.000000000000E+00

KE= 1.906564245666D+03 PE=-1.517667742905D+04 EE= 6.009752238665D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.25

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7586, after 0.7500

Leave Link 502 at Sun Aug 18 15:06:56 2019, MaxMem= 2013265920 cpu: 1670.6

(Enter /home/kira/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 = 179

Leave Link 701 at Sun Aug 18 15:07:12 2019, MaxMem= 2013265920 cpu: 124.3

(Enter /home/kira/g09/l702.exe)

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

Leave Link 702 at Sun Aug 18 15:07:12 2019, MaxMem= 2013265920 cpu: 0.1

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 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= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

Petite list used in FoFCou.

Leave Link 703 at Sun Aug 18 15:08:17 2019, MaxMem= 2013265920 cpu: 517.9

(Enter /home/kira/g09/l716.exe)

Dipole =-2.90202651D-06-1.05340459D-01-4.73399098D-13

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000001119 -0.000001642 -0.000005963

2 6 -0.000000932 0.000006081 -0.000013552

3 7 0.000012089 -0.000008971 -0.000000000

4 6 -0.000000932 0.000006081 0.000013552

5 6 0.000001119 -0.000001642 0.000005963

6 6 0.000018320 -0.000012463 -0.000010486

7 6 -0.000026475 0.000006575 0.000007068

8 7 0.000001407 -0.000008129 -0.000018335

9 6 0.000025195 -0.000000947 0.000005042

10 6 -0.000000810 0.000008300 -0.000005104

11 6 -0.000003834 -0.000002276 -0.000006393

12 6 0.000018320 -0.000012463 0.000010486

13 6 -0.000026475 0.000006575 -0.000007068

14 6 -0.000003834 -0.000002276 0.000006393

15 6 -0.000000810 0.000008300 0.000005104

16 6 0.000025195 -0.000000947 -0.000005042

17 7 0.000001407 -0.000008129 0.000018335

18 6 -0.000014141 -0.000015986 0.000006863

19 6 0.000000865 0.000005061 -0.000012139

20 6 -0.000000169 -0.000002775 -0.000002881

21 6 -0.000000169 -0.000002775 0.000002881

22 6 0.000000865 0.000005061 0.000012139

23 7 -0.000008148 -0.000001615 -0.000000000

24 6 -0.000014141 -0.000015986 -0.000006863

25 6 -0.000003619 0.000015607 0.000006958

26 6 -0.000001271 -0.000002471 0.000001515

27 6 0.000001028 -0.000004306 -0.000003720

28 6 0.000000966 0.000002254 0.000000162

29 6 0.000000045 0.000000474 0.000000333

30 6 -0.000003671 -0.000008261 -0.000002099

31 6 0.000000966 0.000002254 -0.000000162

32 6 0.000001028 -0.000004306 0.000003720

33 6 -0.000001271 -0.000002471 -0.000001515

34 6 -0.000003619 0.000015607 -0.000006958

35 6 -0.000003671 -0.000008261 0.000002099

36 6 0.000000045 0.000000474 -0.000000333

37 6 -0.000000309 0.000017889 0.000004670

38 6 0.000004757 -0.000007704 0.000001250

39 6 -0.000000117 0.000000376 -0.000000478

40 6 -0.000000526 0.000002671 0.000000599

41 6 -0.000001721 -0.000004806 -0.000003950

42 6 0.000004279 -0.000003482 0.000002075

43 6 -0.000000309 0.000017889 -0.000004670

44 6 0.000004757 -0.000007704 -0.000001250

45 6 -0.000000117 0.000000376 0.000000478

46 6 -0.000000526 0.000002671 -0.000000599

47 6 -0.000001721 -0.000004806 0.000003950

48 6 0.000004279 -0.000003482 -0.000002075

49 1 -0.000002720 0.000002366 0.000002234

50 1 -0.000002720 0.000002366 -0.000002234

51 1 -0.000003887 -0.000000821 0.000003707

52 1 0.000001240 -0.000001863 0.000004918

53 1 0.000001240 -0.000001863 -0.000004918

54 1 -0.000003887 -0.000000821 -0.000003707

55 1 0.000001652 0.000004350 0.000003880

56 1 0.000001652 0.000004350 -0.000003880

57 1 0.000000526 -0.000000052 -0.000000893

58 1 -0.000000940 0.000000486 0.000000520

59 1 -0.000000222 0.000000488 0.000000169

60 1 -0.000000324 -0.000000584 0.000001190

61 1 0.000002024 0.000000703 -0.000000804

62 1 -0.000000222 0.000000488 -0.000000169

63 1 -0.000000940 0.000000486 -0.000000520

64 1 0.000000526 -0.000000052 0.000000893

65 1 0.000002024 0.000000703 0.000000804

66 1 -0.000000324 -0.000000584 -0.000001190

67 1 -0.000000581 0.000000583 -0.000001192

68 1 0.000000538 -0.000000499 0.000001205

69 1 0.000000206 0.000000440 0.000000335

70 1 0.000000927 0.000000411 0.000000680

71 1 -0.000000990 0.000000023 0.000000762

72 1 -0.000000581 0.000000583 0.000001192

73 1 0.000000538 -0.000000499 -0.000001205

74 1 0.000000206 0.000000440 -0.000000335

75 1 0.000000927 0.000000411 -0.000000680

76 1 -0.000000990 0.000000023 -0.000000762

77 1 -0.000002070 0.000011227 -0.000000000

78 1 0.000002456 0.000007219 0.000000000

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

Cartesian Forces: Max 0.000026475 RMS 0.000006468

Leave Link 716 at Sun Aug 18 15:08:17 2019, MaxMem= 2013265920 cpu: 0.2

(Enter /home/kira/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 0.000016707 RMS 0.000003359

Search for a local minimum.

Step number 11 out of a maximum of 452

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

RMS Force = .33588D-05 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 3 4 5 6 7

8 9 10 11

DE= -8.72D-08 DEPred=-8.50D-08 R= 1.03D+00

Trust test= 1.03D+00 RLast= 3.83D-03 DXMaxT set to 9.59D-01

ITU= 0 0 1 1 1 0 1 1 1 1 0

Eigenvalues --- 0.00408 0.00786 0.00983 0.00988 0.01022

Eigenvalues --- 0.01550 0.01608 0.01616 0.01632 0.01635

Eigenvalues --- 0.01659 0.01668 0.01723 0.01723 0.01723

Eigenvalues --- 0.01737 0.01747 0.01751 0.01773 0.01791

Eigenvalues --- 0.01802 0.01837 0.01847 0.01856 0.01891

Eigenvalues --- 0.01906 0.01937 0.01943 0.01954 0.01983

Eigenvalues --- 0.02011 0.02020 0.02027 0.02068 0.02068

Eigenvalues --- 0.02070 0.02070 0.02074 0.02088 0.02099

Eigenvalues --- 0.02117 0.02118 0.02119 0.02121 0.02130

Eigenvalues --- 0.02130 0.02132 0.02132 0.02132 0.02138

Eigenvalues --- 0.02160 0.02160 0.02160 0.02161 0.02162

Eigenvalues --- 0.02162 0.02162 0.02172 0.02173 0.02173

Eigenvalues --- 0.02173 0.02181 0.02181 0.02181 0.02184

Eigenvalues --- 0.02186 0.02187 0.02187 0.02187 0.02216

Eigenvalues --- 0.02217 0.02321 0.02590 0.02906 0.04390

Eigenvalues --- 0.15608 0.15951 0.15952 0.15990 0.15997

Eigenvalues --- 0.15997 0.15997 0.15997 0.15998 0.15999

Eigenvalues --- 0.15999 0.15999 0.15999 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16004 0.16006 0.16022 0.16046

Eigenvalues --- 0.21587 0.22000 0.22000 0.22000 0.22000

Eigenvalues --- 0.22000 0.22001 0.22001 0.22100 0.22759

Eigenvalues --- 0.22773 0.22816 0.22936 0.23472 0.23472

Eigenvalues --- 0.23486 0.23654 0.23912 0.24251 0.24734

Eigenvalues --- 0.24855 0.24882 0.24971 0.24984 0.24997

Eigenvalues --- 0.24997 0.24999 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25126 0.25185

Eigenvalues --- 0.26155 0.27910 0.34159 0.34201 0.34206

Eigenvalues --- 0.34581 0.35411 0.35413 0.35413 0.35413

Eigenvalues --- 0.35415 0.35415 0.35416 0.35416 0.35416

Eigenvalues --- 0.35416 0.35416 0.35424 0.35506 0.35508

Eigenvalues --- 0.35509 0.35522 0.35542 0.35546 0.35547

Eigenvalues --- 0.35715 0.36056 0.36058 0.36073 0.36113

Eigenvalues --- 0.36246 0.36250 0.36251 0.36264 0.37119

Eigenvalues --- 0.37159 0.37294 0.37349 0.37716 0.39141

Eigenvalues --- 0.39745 0.39997 0.40261 0.40464 0.40602

Eigenvalues --- 0.40976 0.41782 0.41797 0.41804 0.42030

Eigenvalues --- 0.42091 0.42093 0.42094 0.42202 0.42675

Eigenvalues --- 0.43359 0.44662 0.44975 0.45566 0.45569

Eigenvalues --- 0.45582 0.45586 0.45773 0.45862 0.45902

Eigenvalues --- 0.45923 0.45930 0.45942 0.45948 0.45970

Eigenvalues --- 0.46102 0.46660 0.46660 0.46661 0.46695

Eigenvalues --- 0.47073 0.47079 0.47086 0.47550 0.47900

Eigenvalues --- 0.48191 0.48279 0.49357 0.49434 0.49975

Eigenvalues --- 0.50775 0.50845 0.54730

En-DIIS/RFO-DIIS IScMMF= 0 using points: 11 10 9 8 7

RFO step: Lambda=-1.17267247D-08.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 1.04D-05 SmlDif= 1.00D-05

RMS Error= 0.1016716416D-04 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.07333 -0.02276 -0.08855 0.03272 0.00526

Iteration 1 RMS(Cart)= 0.00019173 RMS(Int)= 0.00000002

Iteration 2 RMS(Cart)= 0.00000005 RMS(Int)= 0.00000002

ITry= 1 IFail=0 DXMaxC= 9.69D-04 DCOld= 1.00D+10 DXMaxT= 9.59D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.36D-08 for atom 62.

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

(Linear) (Quad) (Total)

R1 2.72731 -0.00000 0.00001 0.00000 0.00001 2.72732

R2 2.57358 -0.00000 -0.00001 -0.00000 -0.00001 2.57357

R3 2.03837 -0.00000 0.00000 -0.00000 -0.00000 2.03837

R4 2.61837 -0.00000 -0.00000 -0.00001 -0.00001 2.61836

R5 2.61826 0.00001 -0.00001 0.00002 0.00001 2.61828

R6 2.61837 -0.00000 -0.00000 -0.00001 -0.00001 2.61836

R7 1.90983 0.00000 0.00000 0.00000 0.00000 1.90983

R8 2.72731 -0.00000 0.00001 0.00000 0.00001 2.72732

R9 2.61826 0.00001 -0.00001 0.00002 0.00001 2.61828

R10 2.03837 -0.00000 0.00000 -0.00000 -0.00000 2.03837

R11 2.70314 0.00002 0.00000 0.00005 0.00005 2.70319

R12 2.82090 -0.00001 -0.00000 -0.00002 -0.00003 2.82087

R13 2.59345 -0.00002 -0.00000 -0.00003 -0.00004 2.59341

R14 2.71578 0.00000 0.00000 0.00001 0.00001 2.71579

R15 2.59345 -0.00001 -0.00001 -0.00003 -0.00004 2.59341

R16 2.71579 -0.00000 0.00000 -0.00000 0.00000 2.71579

R17 2.70316 0.00001 0.00000 0.00003 0.00003 2.70319

R18 2.60026 -0.00000 -0.00000 0.00001 0.00001 2.60026

R19 2.04091 -0.00000 -0.00000 -0.00000 -0.00000 2.04090

R20 2.04091 -0.00000 0.00000 -0.00001 -0.00001 2.04090

R21 2.70314 0.00002 0.00000 0.00005 0.00005 2.70319

R22 2.82090 -0.00001 -0.00000 -0.00002 -0.00003 2.82087

R23 2.71578 0.00000 0.00000 0.00001 0.00001 2.71579

R24 2.59345 -0.00002 -0.00000 -0.00003 -0.00004 2.59341

R25 2.60026 -0.00000 -0.00000 0.00001 0.00001 2.60026

R26 2.04091 -0.00000 0.00000 -0.00001 -0.00001 2.04090

R27 2.71579 -0.00000 0.00000 -0.00000 0.00000 2.71579

R28 2.04091 -0.00000 -0.00000 -0.00000 -0.00000 2.04090

R29 2.59345 -0.00001 -0.00001 -0.00003 -0.00004 2.59341

R30 2.70316 0.00001 0.00000 0.00003 0.00003 2.70319

R31 2.61828 0.00000 -0.00000 -0.00000 -0.00000 2.61827

R32 2.82090 -0.00001 -0.00000 -0.00003 -0.00003 2.82087

R33 2.72731 -0.00000 0.00001 -0.00000 0.00000 2.72732

R34 2.61837 -0.00001 -0.00000 -0.00002 -0.00002 2.61836

R35 2.57358 -0.00000 -0.00001 -0.00000 -0.00001 2.57358

R36 2.03836 0.00000 0.00000 0.00000 0.00000 2.03837

R37 2.72731 -0.00000 0.00001 -0.00000 0.00000 2.72732

R38 2.03836 0.00000 0.00000 0.00000 0.00000 2.03837

R39 2.61837 -0.00001 -0.00000 -0.00002 -0.00002 2.61836

R40 2.61828 0.00000 -0.00000 -0.00000 -0.00000 2.61827

R41 1.90983 0.00000 0.00000 0.00000 0.00001 1.90983

R42 2.82090 -0.00001 -0.00000 -0.00003 -0.00003 2.82087

R43 2.64668 -0.00000 0.00000 -0.00001 -0.00001 2.64667

R44 2.64853 0.00001 0.00000 0.00001 0.00002 2.64854

R45 2.63418 0.00000 -0.00000 0.00000 0.00000 2.63418

R46 2.04989 -0.00000 -0.00000 -0.00000 -0.00000 2.04989

R47 2.63377 -0.00000 0.00000 -0.00001 -0.00000 2.63377

R48 2.05087 -0.00000 0.00000 -0.00000 -0.00000 2.05087

R49 2.63635 0.00000 -0.00000 0.00000 0.00000 2.63635

R50 2.05050 -0.00000 -0.00000 -0.00000 -0.00000 2.05050

R51 2.63139 -0.00000 0.00000 -0.00000 -0.00000 2.63139

R52 2.05088 -0.00000 0.00000 -0.00000 -0.00000 2.05088

R53 2.04962 -0.00000 -0.00000 -0.00000 -0.00000 2.04961

R54 2.63377 -0.00000 0.00000 -0.00001 -0.00000 2.63377

R55 2.63635 0.00000 -0.00000 0.00000 0.00000 2.63635

R56 2.05050 -0.00000 -0.00000 -0.00000 -0.00000 2.05050

R57 2.63418 0.00000 -0.00000 0.00000 0.00000 2.63418

R58 2.05087 -0.00000 0.00000 -0.00000 -0.00000 2.05087

R59 2.64668 -0.00000 0.00000 -0.00001 -0.00001 2.64667

R60 2.04989 -0.00000 -0.00000 -0.00000 -0.00000 2.04989

R61 2.64853 0.00001 0.00000 0.00001 0.00002 2.64854

R62 2.63139 -0.00000 0.00000 -0.00000 -0.00000 2.63139

R63 2.04962 -0.00000 -0.00000 -0.00000 -0.00000 2.04961

R64 2.05088 -0.00000 0.00000 -0.00000 -0.00000 2.05088

R65 2.64853 0.00000 0.00000 0.00001 0.00001 2.64854

R66 2.64669 -0.00001 0.00000 -0.00001 -0.00001 2.64667

R67 2.63139 -0.00000 0.00000 -0.00000 -0.00000 2.63139

R68 2.04961 -0.00000 -0.00000 -0.00000 -0.00000 2.04961

R69 2.63634 0.00000 -0.00000 0.00000 0.00000 2.63635

R70 2.05088 -0.00000 0.00000 -0.00000 -0.00000 2.05088

R71 2.63377 -0.00000 0.00000 -0.00000 -0.00000 2.63377

R72 2.05050 -0.00000 -0.00000 -0.00000 -0.00000 2.05050

R73 2.63418 0.00000 -0.00000 0.00000 0.00000 2.63418

R74 2.05087 -0.00000 0.00000 -0.00000 -0.00000 2.05087

R75 2.04989 0.00000 -0.00000 0.00000 0.00000 2.04989

R76 2.64853 0.00000 0.00000 0.00001 0.00001 2.64854

R77 2.64669 -0.00001 0.00000 -0.00001 -0.00001 2.64667

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A3 2.21364 0.00000 0.00000 0.00003 0.00003 2.21367

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A18 2.04758 -0.00001 -0.00000 -0.00002 -0.00002 2.04755

A19 2.19209 -0.00000 0.00000 0.00001 0.00001 2.19210

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A23 1.92996 0.00001 0.00000 0.00001 0.00001 1.92997

A24 2.19208 0.00000 0.00000 0.00002 0.00002 2.19210

A25 2.16114 -0.00001 -0.00001 -0.00002 -0.00003 2.16111

A26 1.85817 -0.00001 -0.00000 -0.00001 -0.00002 1.85815

A27 2.20392 -0.00000 -0.00000 -0.00003 -0.00003 2.20388

A28 2.22101 0.00001 0.00000 0.00005 0.00005 2.22106

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D6 -3.12791 0.00000 0.00001 -0.00000 0.00001 -3.12791

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D10 3.06784 0.00000 0.00019 0.00031 0.00050 3.06835

D11 -3.13904 0.00000 -0.00006 0.00016 0.00010 -3.13894

D12 -0.06217 0.00000 0.00020 0.00037 0.00057 -0.06159

D13 -3.08347 0.00000 -0.00001 -0.00002 -0.00003 -3.08350

D14 0.05612 0.00000 0.00000 -0.00001 -0.00000 0.05612

D15 0.04415 0.00000 -0.00002 -0.00010 -0.00012 0.04403

D16 -3.09945 -0.00000 -0.00001 -0.00008 -0.00009 -3.09953

D17 0.00904 -0.00000 0.00006 -0.00009 -0.00003 0.00900

D18 3.13904 -0.00000 0.00006 -0.00016 -0.00010 3.13894

D19 -3.06784 -0.00000 -0.00019 -0.00031 -0.00050 -3.06835

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D21 -0.00540 0.00000 -0.00004 0.00006 0.00002 -0.00538

D22 3.12290 0.00000 -0.00005 0.00006 0.00001 3.12292

D23 -3.13540 0.00000 -0.00003 0.00012 0.00009 -3.13531

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D25 -0.04415 -0.00000 0.00002 0.00010 0.00012 -0.04403

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D32 -0.11384 -0.00000 0.00001 -0.00008 -0.00007 -0.11391

D33 -1.12661 -0.00000 -0.00003 -0.00000 -0.00003 -1.12664

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D36 -1.12328 -0.00000 -0.00001 -0.00005 -0.00006 -1.12334

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D63 -2.01682 0.00000 0.00004 0.00002 0.00006 -2.01676

D64 1.12328 0.00000 0.00001 0.00005 0.00006 1.12334

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D66 0.02243 -0.00000 -0.00001 -0.00003 -0.00004 0.02238

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D143 3.13346 -0.00000 -0.00000 -0.00001 -0.00001 3.13345

D144 0.00025 -0.00000 -0.00000 -0.00001 -0.00001 0.00024

D145 -0.00101 0.00000 -0.00000 0.00000 0.00000 -0.00101

D146 3.13581 -0.00000 -0.00001 0.00001 -0.00000 3.13581

D147 3.14140 -0.00000 0.00000 -0.00001 -0.00001 3.14139

D148 -0.00497 -0.00000 -0.00001 -0.00000 -0.00001 -0.00498

D149 -0.00008 -0.00000 0.00000 -0.00002 -0.00002 -0.00010

D150 3.13739 -0.00000 -0.00000 -0.00003 -0.00003 3.13736

D151 3.14069 -0.00000 -0.00000 -0.00001 -0.00001 3.14068

D152 -0.00502 -0.00000 -0.00000 -0.00002 -0.00002 -0.00504

D153 -0.00181 0.00000 -0.00000 0.00003 0.00003 -0.00178

D154 3.13321 -0.00000 -0.00001 0.00001 -0.00001 3.13320

D155 -3.13864 0.00000 0.00001 0.00003 0.00003 -3.13861

D156 -0.00363 0.00000 -0.00001 0.00000 -0.00001 -0.00364

D157 -3.13747 -0.00000 -0.00002 -0.00002 -0.00004 -3.13750

D158 0.00559 -0.00000 0.00000 -0.00005 -0.00004 0.00555

D159 0.01067 0.00000 -0.00000 0.00001 0.00000 0.01067

D160 -3.12946 -0.00000 0.00002 -0.00002 -0.00000 -3.12946

D161 3.13635 -0.00000 0.00002 -0.00000 0.00002 3.13637

D162 0.00308 0.00000 0.00002 0.00000 0.00002 0.00311

D163 -0.00670 0.00000 -0.00000 0.00003 0.00002 -0.00667

D164 -3.13997 0.00000 -0.00000 0.00003 0.00003 -3.13994

D165 0.00402 0.00000 0.00000 0.00000 0.00001 0.00403

D166 -3.13346 0.00000 0.00000 0.00001 0.00001 -3.13345

D167 3.13724 -0.00000 0.00000 0.00000 0.00000 3.13724

D168 -0.00025 0.00000 0.00000 0.00001 0.00001 -0.00024

D169 3.13635 -0.00000 0.00001 0.00000 0.00002 3.13637

D170 0.00311 -0.00000 0.00002 -0.00003 -0.00001 0.00310

D171 -0.00670 0.00000 -0.00001 0.00004 0.00003 -0.00667

D172 -3.13995 0.00000 -0.00000 0.00001 0.00001 -3.13994

D173 -3.13748 0.00000 -0.00002 -0.00000 -0.00002 -3.13750

D174 0.01068 -0.00000 -0.00000 -0.00001 -0.00001 0.01067

D175 0.00558 -0.00000 0.00000 -0.00004 -0.00004 0.00555

D176 -3.12944 -0.00000 0.00002 -0.00005 -0.00003 -3.12947

D177 0.00403 -0.00000 0.00001 -0.00001 -0.00001 0.00402

D178 -3.13346 0.00000 0.00001 -0.00000 0.00000 -3.13345

D179 3.13722 0.00000 0.00000 0.00002 0.00002 3.13724

D180 -0.00026 0.00000 0.00000 0.00003 0.00003 -0.00023

D181 -0.00009 -0.00000 -0.00000 -0.00001 -0.00001 -0.00010

D182 3.14068 -0.00000 -0.00000 0.00000 -0.00000 3.14068

D183 3.13738 -0.00000 -0.00000 -0.00002 -0.00002 3.13736

D184 -0.00503 -0.00000 -0.00000 -0.00001 -0.00001 -0.00504

D185 -0.00102 0.00000 -0.00000 0.00001 0.00001 -0.00101

D186 3.13580 0.00000 -0.00001 0.00001 0.00000 3.13581

D187 3.14139 0.00000 -0.00000 -0.00000 -0.00000 3.14139

D188 -0.00497 -0.00000 -0.00001 -0.00000 -0.00001 -0.00498

D189 -0.00179 0.00000 0.00000 0.00002 0.00002 -0.00178

D190 3.13319 0.00000 -0.00001 0.00002 0.00001 3.13320

D191 -3.13864 0.00000 0.00001 0.00001 0.00002 -3.13861

D192 -0.00365 0.00000 -0.00001 0.00002 0.00001 -0.00364

D193 -3.13635 0.00000 -0.00001 -0.00000 -0.00002 -3.13637

D194 -0.00311 0.00000 -0.00002 0.00003 0.00001 -0.00310

D195 0.00670 -0.00000 0.00001 -0.00004 -0.00003 0.00667

D196 3.13995 -0.00000 0.00000 -0.00001 -0.00001 3.13994

D197 3.13748 -0.00000 0.00002 0.00000 0.00002 3.13750

D198 -0.01068 0.00000 0.00000 0.00001 0.00001 -0.01067

D199 -0.00558 0.00000 -0.00000 0.00004 0.00004 -0.00555

D200 3.12944 0.00000 -0.00002 0.00005 0.00003 3.12947

D201 -0.00403 0.00000 -0.00001 0.00001 0.00001 -0.00402

D202 3.13346 -0.00000 -0.00001 0.00000 -0.00000 3.13345

D203 -3.13722 -0.00000 -0.00000 -0.00002 -0.00002 -3.13724

D204 0.00026 -0.00000 -0.00000 -0.00003 -0.00003 0.00023

D205 0.00009 0.00000 0.00000 0.00001 0.00001 0.00010

D206 -3.14068 0.00000 0.00000 -0.00000 0.00000 -3.14068

D207 -3.13738 0.00000 0.00000 0.00002 0.00002 -3.13736

D208 0.00503 0.00000 0.00000 0.00001 0.00001 0.00504

D209 0.00102 -0.00000 0.00000 -0.00001 -0.00001 0.00101

D210 -3.13580 -0.00000 0.00001 -0.00001 -0.00000 -3.13581

D211 -3.14139 -0.00000 0.00000 0.00000 0.00000 -3.14139

D212 0.00497 0.00000 0.00001 0.00000 0.00001 0.00498

D213 0.00179 -0.00000 -0.00000 -0.00002 -0.00002 0.00178

D214 -3.13319 -0.00000 0.00001 -0.00002 -0.00001 -3.13320

D215 3.13864 -0.00000 -0.00001 -0.00001 -0.00002 3.13861

D216 0.00365 -0.00000 0.00001 -0.00002 -0.00001 0.00364

Item Value Threshold Converged?

Maximum Force 0.000017 0.000450 YES

RMS Force 0.000003 0.000300 YES

Maximum Displacement 0.000969 0.001800 YES

RMS Displacement 0.000192 0.001200 YES

Predicted change in Energy=-2.281411D-08

Optimization completed.

-- Stationary point found.

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! Optimized Parameters !

! (Angstroms and Degrees) !

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! Name Definition Value Derivative Info. !

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

! R1 R(1,2) 1.4432 -DE/DX = 0.0 !

! R2 R(1,5) 1.3619 -DE/DX = 0.0 !

! R3 R(1,49) 1.0787 -DE/DX = 0.0 !

! R4 R(2,3) 1.3856 -DE/DX = 0.0 !

! R5 R(2,12) 1.3855 -DE/DX = 0.0 !

! R6 R(3,4) 1.3856 -DE/DX = 0.0 !

! R7 R(3,77) 1.0106 -DE/DX = 0.0 !

! R8 R(4,5) 1.4432 -DE/DX = 0.0 !

! R9 R(4,6) 1.3855 -DE/DX = 0.0 !

! R10 R(5,50) 1.0787 -DE/DX = 0.0 !

! R11 R(6,7) 1.4304 -DE/DX = 0.0 !

! R12 R(6,25) 1.4928 -DE/DX = 0.0 !

! R13 R(7,8) 1.3724 -DE/DX = 0.0 !

! R14 R(7,11) 1.4371 -DE/DX = 0.0 !

! R15 R(8,9) 1.3724 -DE/DX = 0.0 !

! R16 R(9,10) 1.4371 -DE/DX = 0.0 !

! R17 R(9,24) 1.4304 -DE/DX = 0.0 !

! R18 R(10,11) 1.376 -DE/DX = 0.0 !

! R19 R(10,51) 1.08 -DE/DX = 0.0 !

! R20 R(11,52) 1.08 -DE/DX = 0.0 !

! R21 R(12,13) 1.4304 -DE/DX = 0.0 !

! R22 R(12,34) 1.4928 -DE/DX = 0.0 !

! R23 R(13,14) 1.4371 -DE/DX = 0.0 !

! R24 R(13,17) 1.3724 -DE/DX = 0.0 !

! R25 R(14,15) 1.376 -DE/DX = 0.0 !

! R26 R(14,53) 1.08 -DE/DX = 0.0 !

! R27 R(15,16) 1.4371 -DE/DX = 0.0 !

! R28 R(15,54) 1.08 -DE/DX = 0.0 !

! R29 R(16,17) 1.3724 -DE/DX = 0.0 !

! R30 R(16,18) 1.4304 -DE/DX = 0.0 !

! R31 R(18,19) 1.3855 -DE/DX = 0.0 !

! R32 R(18,43) 1.4928 -DE/DX = 0.0 !

! R33 R(19,20) 1.4432 -DE/DX = 0.0 !

! R34 R(19,23) 1.3856 -DE/DX = 0.0 !

! R35 R(20,21) 1.3619 -DE/DX = 0.0 !

! R36 R(20,55) 1.0787 -DE/DX = 0.0 !

! R37 R(21,22) 1.4432 -DE/DX = 0.0 !

! R38 R(21,56) 1.0787 -DE/DX = 0.0 !

! R39 R(22,23) 1.3856 -DE/DX = 0.0 !

! R40 R(22,24) 1.3855 -DE/DX = 0.0 !

! R41 R(23,78) 1.0106 -DE/DX = 0.0 !

! R42 R(24,37) 1.4928 -DE/DX = 0.0 !

! R43 R(25,26) 1.4006 -DE/DX = 0.0 !

! R44 R(25,30) 1.4015 -DE/DX = 0.0 !

! R45 R(26,27) 1.3939 -DE/DX = 0.0 !

! R46 R(26,57) 1.0848 -DE/DX = 0.0 !

! R47 R(27,28) 1.3937 -DE/DX = 0.0 !

! R48 R(27,58) 1.0853 -DE/DX = 0.0 !

! R49 R(28,29) 1.3951 -DE/DX = 0.0 !

! R50 R(28,59) 1.0851 -DE/DX = 0.0 !

! R51 R(29,30) 1.3925 -DE/DX = 0.0 !

! R52 R(29,60) 1.0853 -DE/DX = 0.0 !

! R53 R(30,61) 1.0846 -DE/DX = 0.0 !

! R54 R(31,32) 1.3937 -DE/DX = 0.0 !

! R55 R(31,36) 1.3951 -DE/DX = 0.0 !

! R56 R(31,62) 1.0851 -DE/DX = 0.0 !

! R57 R(32,33) 1.3939 -DE/DX = 0.0 !

! R58 R(32,63) 1.0853 -DE/DX = 0.0 !

! R59 R(33,34) 1.4006 -DE/DX = 0.0 !

! R60 R(33,64) 1.0848 -DE/DX = 0.0 !

! R61 R(34,35) 1.4015 -DE/DX = 0.0 !

! R62 R(35,36) 1.3925 -DE/DX = 0.0 !

! R63 R(35,65) 1.0846 -DE/DX = 0.0 !

! R64 R(36,66) 1.0853 -DE/DX = 0.0 !

! R65 R(37,38) 1.4015 -DE/DX = 0.0 !

! R66 R(37,42) 1.4006 -DE/DX = 0.0 !

! R67 R(38,39) 1.3925 -DE/DX = 0.0 !

! R68 R(38,67) 1.0846 -DE/DX = 0.0 !

! R69 R(39,40) 1.3951 -DE/DX = 0.0 !

! R70 R(39,68) 1.0853 -DE/DX = 0.0 !

! R71 R(40,41) 1.3937 -DE/DX = 0.0 !

! R72 R(40,69) 1.0851 -DE/DX = 0.0 !

! R73 R(41,42) 1.3939 -DE/DX = 0.0 !

! R74 R(41,70) 1.0853 -DE/DX = 0.0 !

! R75 R(42,71) 1.0848 -DE/DX = 0.0 !

! R76 R(43,44) 1.4015 -DE/DX = 0.0 !

! R77 R(43,48) 1.4006 -DE/DX = 0.0 !

! R78 R(44,45) 1.3925 -DE/DX = 0.0 !

! R79 R(44,72) 1.0846 -DE/DX = 0.0 !

! R80 R(45,46) 1.3951 -DE/DX = 0.0 !

! R81 R(45,73) 1.0853 -DE/DX = 0.0 !

! R82 R(46,47) 1.3937 -DE/DX = 0.0 !

! R83 R(46,74) 1.0851 -DE/DX = 0.0 !

! R84 R(47,48) 1.3939 -DE/DX = 0.0 !

! R85 R(47,75) 1.0853 -DE/DX = 0.0 !

! R86 R(48,76) 1.0848 -DE/DX = 0.0 !

! A1 A(2,1,5) 108.6377 -DE/DX = 0.0 !

! A2 A(2,1,49) 124.5249 -DE/DX = 0.0 !

! A3 A(5,1,49) 126.8324 -DE/DX = 0.0 !

! A4 A(1,2,3) 105.8406 -DE/DX = 0.0 !

! A5 A(1,2,12) 127.101 -DE/DX = 0.0 !

! A6 A(3,2,12) 127.0548 -DE/DX = 0.0 !

! A7 A(2,3,4) 111.0407 -DE/DX = 0.0 !

! A8 A(2,3,77) 124.4236 -DE/DX = 0.0 !

! A9 A(4,3,77) 124.4236 -DE/DX = 0.0 !

! A10 A(3,4,5) 105.8406 -DE/DX = 0.0 !

! A11 A(3,4,6) 127.0548 -DE/DX = 0.0 !

! A12 A(5,4,6) 127.101 -DE/DX = 0.0 !

! A13 A(1,5,4) 108.6377 -DE/DX = 0.0 !

! A14 A(1,5,50) 126.8324 -DE/DX = 0.0 !

! A15 A(4,5,50) 124.5249 -DE/DX = 0.0 !

! A16 A(4,6,7) 125.6261 -DE/DX = 0.0 !

! A17 A(4,6,25) 117.0564 -DE/DX = 0.0 !

! A18 A(7,6,25) 117.3175 -DE/DX = 0.0 !

! A19 A(6,7,8) 125.5975 -DE/DX = 0.0 !

! A20 A(6,7,11) 123.8231 -DE/DX = 0.0 !

! A21 A(8,7,11) 110.5792 -DE/DX = 0.0 !

! A22 A(7,8,9) 105.9004 -DE/DX = 0.0 !

! A23 A(8,9,10) 110.5786 -DE/DX = 0.0 !

! A24 A(8,9,24) 125.5968 -DE/DX = 0.0 !

! A25 A(10,9,24) 123.8243 -DE/DX = 0.0 !

! A26 A(9,10,11) 106.4653 -DE/DX = 0.0 !

! A27 A(9,10,51) 126.2752 -DE/DX = 0.0 !

! A28 A(11,10,51) 127.2544 -DE/DX = 0.0 !

! A29 A(7,11,10) 106.4648 -DE/DX = 0.0 !

! A30 A(7,11,52) 126.2751 -DE/DX = 0.0 !

! A31 A(10,11,52) 127.2551 -DE/DX = 0.0 !

! A32 A(2,12,13) 125.6261 -DE/DX = 0.0 !

! A33 A(2,12,34) 117.0564 -DE/DX = 0.0 !

! A34 A(13,12,34) 117.3175 -DE/DX = 0.0 !

! A35 A(12,13,14) 123.8231 -DE/DX = 0.0 !

! A36 A(12,13,17) 125.5975 -DE/DX = 0.0 !

! A37 A(14,13,17) 110.5792 -DE/DX = 0.0 !

! A38 A(13,14,15) 106.4648 -DE/DX = 0.0 !

! A39 A(13,14,53) 126.2751 -DE/DX = 0.0 !

! A40 A(15,14,53) 127.2551 -DE/DX = 0.0 !

! A41 A(14,15,16) 106.4653 -DE/DX = 0.0 !

! A42 A(14,15,54) 127.2544 -DE/DX = 0.0 !

! A43 A(16,15,54) 126.2752 -DE/DX = 0.0 !

! A44 A(15,16,17) 110.5786 -DE/DX = 0.0 !

! A45 A(15,16,18) 123.8243 -DE/DX = 0.0 !

! A46 A(17,16,18) 125.5968 -DE/DX = 0.0 !

! A47 A(13,17,16) 105.9004 -DE/DX = 0.0 !

! A48 A(16,18,19) 125.6257 -DE/DX = 0.0 !

! A49 A(16,18,43) 117.3177 -DE/DX = 0.0 !

! A50 A(19,18,43) 117.0564 -DE/DX = 0.0 !

! A51 A(18,19,20) 127.1011 -DE/DX = 0.0 !

! A52 A(18,19,23) 127.0553 -DE/DX = 0.0 !

! A53 A(20,19,23) 105.8398 -DE/DX = 0.0 !

! A54 A(19,20,21) 108.638 -DE/DX = 0.0 !

! A55 A(19,20,55) 124.5248 -DE/DX = 0.0 !

! A56 A(21,20,55) 126.8322 -DE/DX = 0.0 !

! A57 A(20,21,22) 108.638 -DE/DX = 0.0 !

! A58 A(20,21,56) 126.8322 -DE/DX = 0.0 !

! A59 A(22,21,56) 124.5248 -DE/DX = 0.0 !

! A60 A(21,22,23) 105.8398 -DE/DX = 0.0 !

! A61 A(21,22,24) 127.1011 -DE/DX = 0.0 !

! A62 A(23,22,24) 127.0553 -DE/DX = 0.0 !

! A63 A(19,23,22) 111.0416 -DE/DX = 0.0 !

! A64 A(19,23,78) 124.424 -DE/DX = 0.0 !

! A65 A(22,23,78) 124.424 -DE/DX = 0.0 !

! A66 A(9,24,22) 125.6257 -DE/DX = 0.0 !

! A67 A(9,24,37) 117.3177 -DE/DX = 0.0 !

! A68 A(22,24,37) 117.0564 -DE/DX = 0.0 !

! A69 A(6,25,26) 121.0553 -DE/DX = 0.0 !

! A70 A(6,25,30) 120.5485 -DE/DX = 0.0 !

! A71 A(26,25,30) 118.3961 -DE/DX = 0.0 !

! A72 A(25,26,27) 120.8546 -DE/DX = 0.0 !

! A73 A(25,26,57) 119.2758 -DE/DX = 0.0 !

! A74 A(27,26,57) 119.8685 -DE/DX = 0.0 !

! A75 A(26,27,28) 120.1707 -DE/DX = 0.0 !

! A76 A(26,27,58) 119.7045 -DE/DX = 0.0 !

! A77 A(28,27,58) 120.1243 -DE/DX = 0.0 !

! A78 A(27,28,29) 119.5388 -DE/DX = 0.0 !

! A79 A(27,28,59) 120.2418 -DE/DX = 0.0 !

! A80 A(29,28,59) 120.2193 -DE/DX = 0.0 !

! A81 A(28,29,30) 120.1787 -DE/DX = 0.0 !

! A82 A(28,29,60) 120.095 -DE/DX = 0.0 !

! A83 A(30,29,60) 119.7259 -DE/DX = 0.0 !

! A84 A(25,30,29) 120.8602 -DE/DX = 0.0 !

! A85 A(25,30,61) 119.2639 -DE/DX = 0.0 !

! A86 A(29,30,61) 119.8743 -DE/DX = 0.0 !

! A87 A(32,31,36) 119.5388 -DE/DX = 0.0 !

! A88 A(32,31,62) 120.2418 -DE/DX = 0.0 !

! A89 A(36,31,62) 120.2193 -DE/DX = 0.0 !

! A90 A(31,32,33) 120.1707 -DE/DX = 0.0 !

! A91 A(31,32,63) 120.1243 -DE/DX = 0.0 !

! A92 A(33,32,63) 119.7045 -DE/DX = 0.0 !

! A93 A(32,33,34) 120.8546 -DE/DX = 0.0 !

! A94 A(32,33,64) 119.8685 -DE/DX = 0.0 !

! A95 A(34,33,64) 119.2758 -DE/DX = 0.0 !

! A96 A(12,34,33) 121.0553 -DE/DX = 0.0 !

! A97 A(12,34,35) 120.5485 -DE/DX = 0.0 !

! A98 A(33,34,35) 118.3961 -DE/DX = 0.0 !

! A99 A(34,35,36) 120.8602 -DE/DX = 0.0 !

! A100 A(34,35,65) 119.2639 -DE/DX = 0.0 !

! A101 A(36,35,65) 119.8743 -DE/DX = 0.0 !

! A102 A(31,36,35) 120.1787 -DE/DX = 0.0 !

! A103 A(31,36,66) 120.095 -DE/DX = 0.0 !

! A104 A(35,36,66) 119.7259 -DE/DX = 0.0 !

! A105 A(24,37,38) 120.5494 -DE/DX = 0.0 !

! A106 A(24,37,42) 121.0549 -DE/DX = 0.0 !

! A107 A(38,37,42) 118.3957 -DE/DX = 0.0 !

! A108 A(37,38,39) 120.8603 -DE/DX = 0.0 !

! A109 A(37,38,67) 119.2639 -DE/DX = 0.0 !

! A110 A(39,38,67) 119.8741 -DE/DX = 0.0 !

! A111 A(38,39,40) 120.1788 -DE/DX = 0.0 !

! A112 A(38,39,68) 119.7259 -DE/DX = 0.0 !

! A113 A(40,39,68) 120.0949 -DE/DX = 0.0 !

! A114 A(39,40,41) 119.5387 -DE/DX = 0.0 !

! A115 A(39,40,69) 120.2194 -DE/DX = 0.0 !

! A116 A(41,40,69) 120.2419 -DE/DX = 0.0 !

! A117 A(40,41,42) 120.1707 -DE/DX = 0.0 !

! A118 A(40,41,70) 120.1243 -DE/DX = 0.0 !

! A119 A(42,41,70) 119.7045 -DE/DX = 0.0 !

! A120 A(37,42,41) 120.8548 -DE/DX = 0.0 !

! A121 A(37,42,71) 119.2758 -DE/DX = 0.0 !

! A122 A(41,42,71) 119.8683 -DE/DX = 0.0 !

! A123 A(18,43,44) 120.5494 -DE/DX = 0.0 !

! A124 A(18,43,48) 121.0549 -DE/DX = 0.0 !

! A125 A(44,43,48) 118.3957 -DE/DX = 0.0 !

! A126 A(43,44,45) 120.8603 -DE/DX = 0.0 !

! A127 A(43,44,72) 119.2639 -DE/DX = 0.0 !

! A128 A(45,44,72) 119.8741 -DE/DX = 0.0 !

! A129 A(44,45,46) 120.1788 -DE/DX = 0.0 !

! A130 A(44,45,73) 119.7259 -DE/DX = 0.0 !

! A131 A(46,45,73) 120.0949 -DE/DX = 0.0 !

! A132 A(45,46,47) 119.5387 -DE/DX = 0.0 !

! A133 A(45,46,74) 120.2194 -DE/DX = 0.0 !

! A134 A(47,46,74) 120.2419 -DE/DX = 0.0 !

! A135 A(46,47,48) 120.1707 -DE/DX = 0.0 !

! A136 A(46,47,75) 120.1243 -DE/DX = 0.0 !

! A137 A(48,47,75) 119.7045 -DE/DX = 0.0 !

! A138 A(43,48,47) 120.8548 -DE/DX = 0.0 !

! A139 A(43,48,76) 119.2758 -DE/DX = 0.0 !

! A140 A(47,48,76) 119.8683 -DE/DX = 0.0 !

! D1 D(5,1,2,3) 0.3093 -DE/DX = 0.0 !

! D2 D(5,1,2,12) 179.6451 -DE/DX = 0.0 !

! D3 D(49,1,2,3) -178.9292 -DE/DX = 0.0 !

! D4 D(49,1,2,12) 0.4065 -DE/DX = 0.0 !

! D5 D(2,1,5,4) 0.0 -DE/DX = 0.0 !

! D6 D(2,1,5,50) -179.2162 -DE/DX = 0.0 !

! D7 D(49,1,5,4) 179.2162 -DE/DX = 0.0 !

! D8 D(49,1,5,50) 0.0 -DE/DX = 0.0 !

! D9 D(1,2,3,4) -0.5177 -DE/DX = 0.0 !

! D10 D(1,2,3,77) 175.7744 -DE/DX = 0.0 !

! D11 D(12,2,3,4) -179.8539 -DE/DX = 0.0 !

! D12 D(12,2,3,77) -3.5618 -DE/DX = 0.0 !

! D13 D(1,2,12,13) -176.6697 -DE/DX = 0.0 !

! D14 D(1,2,12,34) 3.2156 -DE/DX = 0.0 !

! D15 D(3,2,12,13) 2.5296 -DE/DX = 0.0 !

! D16 D(3,2,12,34) -177.5851 -DE/DX = 0.0 !

! D17 D(2,3,4,5) 0.5177 -DE/DX = 0.0 !

! D18 D(2,3,4,6) 179.8539 -DE/DX = 0.0 !

! D19 D(77,3,4,5) -175.7744 -DE/DX = 0.0 !

! D20 D(77,3,4,6) 3.5618 -DE/DX = 0.0 !

! D21 D(3,4,5,1) -0.3093 -DE/DX = 0.0 !

! D22 D(3,4,5,50) 178.9292 -DE/DX = 0.0 !

! D23 D(6,4,5,1) -179.6451 -DE/DX = 0.0 !

! D24 D(6,4,5,50) -0.4065 -DE/DX = 0.0 !

! D25 D(3,4,6,7) -2.5296 -DE/DX = 0.0 !

! D26 D(3,4,6,25) 177.5851 -DE/DX = 0.0 !

! D27 D(5,4,6,7) 176.6697 -DE/DX = 0.0 !

! D28 D(5,4,6,25) -3.2156 -DE/DX = 0.0 !

! D29 D(4,6,7,8) -6.2259 -DE/DX = 0.0 !

! D30 D(4,6,7,11) 173.5924 -DE/DX = 0.0 !

! D31 D(25,6,7,8) 173.6591 -DE/DX = 0.0 !

! D32 D(25,6,7,11) -6.5226 -DE/DX = 0.0 !

! D33 D(4,6,25,26) -64.5499 -DE/DX = 0.0 !

! D34 D(4,6,25,30) 115.536 -DE/DX = 0.0 !

! D35 D(7,6,25,26) 115.5551 -DE/DX = 0.0 !

! D36 D(7,6,25,30) -64.3591 -DE/DX = 0.0 !

! D37 D(6,7,8,9) -179.0952 -DE/DX = 0.0 !

! D38 D(11,7,8,9) 1.066 -DE/DX = 0.0 !

! D39 D(6,7,11,10) 179.486 -DE/DX = 0.0 !

! D40 D(6,7,11,52) -1.2851 -DE/DX = 0.0 !

! D41 D(8,7,11,10) -0.6718 -DE/DX = 0.0 !

! D42 D(8,7,11,52) 178.557 -DE/DX = 0.0 !

! D43 D(7,8,9,10) -1.064 -DE/DX = 0.0 !

! D44 D(7,8,9,24) 179.0944 -DE/DX = 0.0 !

! D45 D(8,9,10,11) 0.6664 -DE/DX = 0.0 !

! D46 D(8,9,10,51) -178.5583 -DE/DX = 0.0 !

! D47 D(24,9,10,11) -179.4887 -DE/DX = 0.0 !

! D48 D(24,9,10,51) 1.2867 -DE/DX = 0.0 !

! D49 D(8,9,24,22) 6.2242 -DE/DX = 0.0 !

! D50 D(8,9,24,37) -173.6581 -DE/DX = 0.0 !

! D51 D(10,9,24,22) -173.5972 -DE/DX = 0.0 !

! D52 D(10,9,24,37) 6.5204 -DE/DX = 0.0 !

! D53 D(9,10,11,7) 0.0032 -DE/DX = 0.0 !

! D54 D(9,10,11,52) -179.2158 -DE/DX = 0.0 !

! D55 D(51,10,11,7) 179.2178 -DE/DX = 0.0 !

! D56 D(51,10,11,52) -0.0011 -DE/DX = 0.0 !

! D57 D(2,12,13,14) -173.5924 -DE/DX = 0.0 !

! D58 D(2,12,13,17) 6.2259 -DE/DX = 0.0 !

! D59 D(34,12,13,14) 6.5226 -DE/DX = 0.0 !

! D60 D(34,12,13,17) -173.6591 -DE/DX = 0.0 !

! D61 D(2,12,34,33) 64.5499 -DE/DX = 0.0 !

! D62 D(2,12,34,35) -115.536 -DE/DX = 0.0 !

! D63 D(13,12,34,33) -115.5551 -DE/DX = 0.0 !

! D64 D(13,12,34,35) 64.3591 -DE/DX = 0.0 !

! D65 D(12,13,14,15) -179.486 -DE/DX = 0.0 !

! D66 D(12,13,14,53) 1.2851 -DE/DX = 0.0 !

! D67 D(17,13,14,15) 0.6718 -DE/DX = 0.0 !

! D68 D(17,13,14,53) -178.557 -DE/DX = 0.0 !

! D69 D(12,13,17,16) 179.0952 -DE/DX = 0.0 !

! D70 D(14,13,17,16) -1.066 -DE/DX = 0.0 !

! D71 D(13,14,15,16) -0.0032 -DE/DX = 0.0 !

! D72 D(13,14,15,54) -179.2178 -DE/DX = 0.0 !

! D73 D(53,14,15,16) 179.2158 -DE/DX = 0.0 !

! D74 D(53,14,15,54) 0.0011 -DE/DX = 0.0 !

! D75 D(14,15,16,17) -0.6664 -DE/DX = 0.0 !

! D76 D(14,15,16,18) 179.4887 -DE/DX = 0.0 !

! D77 D(54,15,16,17) 178.5583 -DE/DX = 0.0 !

! D78 D(54,15,16,18) -1.2867 -DE/DX = 0.0 !

! D79 D(15,16,17,13) 1.064 -DE/DX = 0.0 !

! D80 D(18,16,17,13) -179.0944 -DE/DX = 0.0 !

! D81 D(15,16,18,19) 173.5972 -DE/DX = 0.0 !

! D82 D(15,16,18,43) -6.5204 -DE/DX = 0.0 !

! D83 D(17,16,18,19) -6.2242 -DE/DX = 0.0 !

! D84 D(17,16,18,43) 173.6581 -DE/DX = 0.0 !

! D85 D(16,18,19,20) 176.6644 -DE/DX = 0.0 !

! D86 D(16,18,19,23) -2.5323 -DE/DX = 0.0 !

! D87 D(43,18,19,20) -3.2182 -DE/DX = 0.0 !

! D88 D(43,18,19,23) 177.5851 -DE/DX = 0.0 !

! D89 D(16,18,43,44) -64.3647 -DE/DX = 0.0 !

! D90 D(16,18,43,48) 115.5494 -DE/DX = 0.0 !

! D91 D(19,18,43,44) 115.5279 -DE/DX = 0.0 !

! D92 D(19,18,43,48) -64.558 -DE/DX = 0.0 !

! D93 D(18,19,20,21) -179.6456 -DE/DX = 0.0 !

! D94 D(18,19,20,55) -0.4115 -DE/DX = 0.0 !

! D95 D(23,19,20,21) -0.312 -DE/DX = 0.0 !

! D96 D(23,19,20,55) 178.9221 -DE/DX = 0.0 !

! D97 D(18,19,23,22) 179.8563 -DE/DX = 0.0 !

! D98 D(18,19,23,78) 3.5384 -DE/DX = 0.0 !

! D99 D(20,19,23,22) 0.5223 -DE/DX = 0.0 !

! D100 D(20,19,23,78) -175.7956 -DE/DX = 0.0 !

! D101 D(19,20,21,22) 0.0 -DE/DX = 0.0 !

! D102 D(19,20,21,56) 179.2117 -DE/DX = 0.0 !

! D103 D(55,20,21,22) -179.2117 -DE/DX = 0.0 !

! D104 D(55,20,21,56) 0.0 -DE/DX = 0.0 !

! D105 D(20,21,22,23) 0.312 -DE/DX = 0.0 !

! D106 D(20,21,22,24) 179.6456 -DE/DX = 0.0 !

! D107 D(56,21,22,23) -178.9221 -DE/DX = 0.0 !

! D108 D(56,21,22,24) 0.4115 -DE/DX = 0.0 !

! D109 D(21,22,23,19) -0.5223 -DE/DX = 0.0 !

! D110 D(21,22,23,78) 175.7956 -DE/DX = 0.0 !

! D111 D(24,22,23,19) -179.8563 -DE/DX = 0.0 !

! D112 D(24,22,23,78) -3.5384 -DE/DX = 0.0 !

! D113 D(21,22,24,9) -176.6644 -DE/DX = 0.0 !

! D114 D(21,22,24,37) 3.2182 -DE/DX = 0.0 !

! D115 D(23,22,24,9) 2.5323 -DE/DX = 0.0 !

! D116 D(23,22,24,37) -177.5851 -DE/DX = 0.0 !

! D117 D(9,24,37,38) 64.3647 -DE/DX = 0.0 !

! D118 D(9,24,37,42) -115.5494 -DE/DX = 0.0 !

! D119 D(22,24,37,38) -115.5279 -DE/DX = 0.0 !

! D120 D(22,24,37,42) 64.558 -DE/DX = 0.0 !

! D121 D(6,25,26,27) 179.7637 -DE/DX = 0.0 !

! D122 D(6,25,26,57) -0.6111 -DE/DX = 0.0 !

! D123 D(30,25,26,27) -0.3204 -DE/DX = 0.0 !

! D124 D(30,25,26,57) 179.3048 -DE/DX = 0.0 !

! D125 D(6,25,30,29) -179.6999 -DE/DX = 0.0 !

! D126 D(6,25,30,61) -0.1767 -DE/DX = 0.0 !

! D127 D(26,25,30,29) 0.3837 -DE/DX = 0.0 !

! D128 D(26,25,30,61) 179.9069 -DE/DX = 0.0 !

! D129 D(25,26,27,28) 0.1034 -DE/DX = 0.0 !

! D130 D(25,26,27,58) 179.8311 -DE/DX = 0.0 !

! D131 D(57,26,27,28) -179.5195 -DE/DX = 0.0 !

! D132 D(57,26,27,58) 0.2082 -DE/DX = 0.0 !

! D133 D(26,27,28,29) 0.058 -DE/DX = 0.0 !

! D134 D(26,27,28,59) -179.9888 -DE/DX = 0.0 !

! D135 D(58,27,28,29) -179.6685 -DE/DX = 0.0 !

! D136 D(58,27,28,59) 0.2847 -DE/DX = 0.0 !

! D137 D(27,28,29,30) 0.0048 -DE/DX = 0.0 !

! D138 D(27,28,29,60) -179.7589 -DE/DX = 0.0 !

! D139 D(59,28,29,30) -179.9484 -DE/DX = 0.0 !

! D140 D(59,28,29,60) 0.2879 -DE/DX = 0.0 !

! D141 D(28,29,30,25) -0.2303 -DE/DX = 0.0 !

! D142 D(28,29,30,61) -179.7506 -DE/DX = 0.0 !

! D143 D(60,29,30,25) 179.5343 -DE/DX = 0.0 !

! D144 D(60,29,30,61) 0.014 -DE/DX = 0.0 !

! D145 D(36,31,32,33) -0.058 -DE/DX = 0.0 !

! D146 D(36,31,32,63) 179.6685 -DE/DX = 0.0 !

! D147 D(62,31,32,33) 179.9888 -DE/DX = 0.0 !

! D148 D(62,31,32,63) -0.2847 -DE/DX = 0.0 !

! D149 D(32,31,36,35) -0.0048 -DE/DX = 0.0 !

! D150 D(32,31,36,66) 179.7589 -DE/DX = 0.0 !

! D151 D(62,31,36,35) 179.9484 -DE/DX = 0.0 !

! D152 D(62,31,36,66) -0.2879 -DE/DX = 0.0 !

! D153 D(31,32,33,34) -0.1034 -DE/DX = 0.0 !

! D154 D(31,32,33,64) 179.5195 -DE/DX = 0.0 !

! D155 D(63,32,33,34) -179.8311 -DE/DX = 0.0 !

! D156 D(63,32,33,64) -0.2082 -DE/DX = 0.0 !

! D157 D(32,33,34,12) -179.7637 -DE/DX = 0.0 !

! D158 D(32,33,34,35) 0.3204 -DE/DX = 0.0 !

! D159 D(64,33,34,12) 0.6111 -DE/DX = 0.0 !

! D160 D(64,33,34,35) -179.3048 -DE/DX = 0.0 !

! D161 D(12,34,35,36) 179.6999 -DE/DX = 0.0 !

! D162 D(12,34,35,65) 0.1767 -DE/DX = 0.0 !

! D163 D(33,34,35,36) -0.3837 -DE/DX = 0.0 !

! D164 D(33,34,35,65) -179.9069 -DE/DX = 0.0 !

! D165 D(34,35,36,31) 0.2303 -DE/DX = 0.0 !

! D166 D(34,35,36,66) -179.5343 -DE/DX = 0.0 !

! D167 D(65,35,36,31) 179.7506 -DE/DX = 0.0 !

! D168 D(65,35,36,66) -0.014 -DE/DX = 0.0 !

! D169 D(24,37,38,39) 179.6997 -DE/DX = 0.0 !

! D170 D(24,37,38,67) 0.178 -DE/DX = 0.0 !

! D171 D(42,37,38,39) -0.3839 -DE/DX = 0.0 !

! D172 D(42,37,38,67) -179.9056 -DE/DX = 0.0 !

! D173 D(24,37,42,41) -179.7642 -DE/DX = 0.0 !

! D174 D(24,37,42,71) 0.6121 -DE/DX = 0.0 !

! D175 D(38,37,42,41) 0.3199 -DE/DX = 0.0 !

! D176 D(38,37,42,71) -179.3038 -DE/DX = 0.0 !

! D177 D(37,38,39,40) 0.2309 -DE/DX = 0.0 !

! D178 D(37,38,39,68) -179.5338 -DE/DX = 0.0 !

! D179 D(67,38,39,40) 179.7497 -DE/DX = 0.0 !

! D180 D(67,38,39,68) -0.015 -DE/DX = 0.0 !

! D181 D(38,39,40,41) -0.0052 -DE/DX = 0.0 !

! D182 D(38,39,40,69) 179.9479 -DE/DX = 0.0 !

! D183 D(68,39,40,41) 179.7587 -DE/DX = 0.0 !

! D184 D(68,39,40,69) -0.2883 -DE/DX = 0.0 !

! D185 D(39,40,41,42) -0.0583 -DE/DX = 0.0 !

! D186 D(39,40,41,70) 179.6684 -DE/DX = 0.0 !

! D187 D(69,40,41,42) 179.9887 -DE/DX = 0.0 !

! D188 D(69,40,41,70) -0.2847 -DE/DX = 0.0 !

! D189 D(40,41,42,37) -0.1027 -DE/DX = 0.0 !

! D190 D(40,41,42,71) 179.5187 -DE/DX = 0.0 !

! D191 D(70,41,42,37) -179.8306 -DE/DX = 0.0 !

! D192 D(70,41,42,71) -0.2091 -DE/DX = 0.0 !

! D193 D(18,43,44,45) -179.6997 -DE/DX = 0.0 !

! D194 D(18,43,44,72) -0.178 -DE/DX = 0.0 !

! D195 D(48,43,44,45) 0.3839 -DE/DX = 0.0 !

! D196 D(48,43,44,72) 179.9056 -DE/DX = 0.0 !

! D197 D(18,43,48,47) 179.7642 -DE/DX = 0.0 !

! D198 D(18,43,48,76) -0.6121 -DE/DX = 0.0 !

! D199 D(44,43,48,47) -0.3199 -DE/DX = 0.0 !

! D200 D(44,43,48,76) 179.3038 -DE/DX = 0.0 !

! D201 D(43,44,45,46) -0.2309 -DE/DX = 0.0 !

! D202 D(43,44,45,73) 179.5338 -DE/DX = 0.0 !

! D203 D(72,44,45,46) -179.7497 -DE/DX = 0.0 !

! D204 D(72,44,45,73) 0.015 -DE/DX = 0.0 !

! D205 D(44,45,46,47) 0.0052 -DE/DX = 0.0 !

! D206 D(44,45,46,74) -179.9479 -DE/DX = 0.0 !

! D207 D(73,45,46,47) -179.7587 -DE/DX = 0.0 !

! D208 D(73,45,46,74) 0.2883 -DE/DX = 0.0 !

! D209 D(45,46,47,48) 0.0583 -DE/DX = 0.0 !

! D210 D(45,46,47,75) -179.6684 -DE/DX = 0.0 !

! D211 D(74,46,47,48) -179.9887 -DE/DX = 0.0 !

! D212 D(74,46,47,75) 0.2847 -DE/DX = 0.0 !

! D213 D(46,47,48,43) 0.1027 -DE/DX = 0.0 !

! D214 D(46,47,48,76) -179.5187 -DE/DX = 0.0 !

! D215 D(75,47,48,43) 179.8306 -DE/DX = 0.0 !

! D216 D(75,47,48,76) 0.2091 -DE/DX = 0.0 !

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

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Largest change from initial coordinates is atom 58 1.707 Angstoms.

Leave Link 103 at Sun Aug 18 15:08:17 2019, MaxMem= 2013265920 cpu: 1.4

(Enter /home/kira/g09/l202.exe)

Stoichiometry C44H30N4(1-,2)

Framework group CS[SG(H2N2),X(C44H28N2)]

Deg. of freedom 116

Full point group CS NOp 2

RotChk: IX=3 Diff= 3.21D-14

Largest Abelian subgroup CS NOp 2

Largest concise Abelian subgroup CS NOp 2

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 4.259425 -0.136212 0.680941

2 6 0 2.898045 -0.006510 1.142174

3 7 0 2.116534 0.060719 -0.000000

4 6 0 2.898045 -0.006510 -1.142174

5 6 0 4.259425 -0.136212 -0.680941

6 6 0 2.460576 0.028292 -2.456362

7 6 0 1.095329 0.090736 -2.878694

8 7 0 -0.000001 0.005126 -2.056266

9 6 0 -1.095320 0.090756 -2.878707

10 6 0 -0.687976 0.258285 -4.246682

11 6 0 0.688020 0.258320 -4.246668

12 6 0 2.460576 0.028292 2.456362

13 6 0 1.095329 0.090736 2.878694

14 6 0 0.688020 0.258320 4.246668

15 6 0 -0.687976 0.258285 4.246682

16 6 0 -1.095320 0.090756 2.878707

17 7 0 -0.000001 0.005126 2.056266

18 6 0 -2.460574 0.028318 2.456376

19 6 0 -2.898039 -0.006527 1.142180

20 6 0 -4.259409 -0.136332 0.680940

21 6 0 -4.259409 -0.136332 -0.680940

22 6 0 -2.898039 -0.006527 -1.142180

23 7 0 -2.116538 0.060696 0.000000

24 6 0 -2.460574 0.028318 -2.456376

25 6 0 3.506228 -0.004777 -3.521177

26 6 0 4.426960 1.041117 -3.662366

27 6 0 5.404782 1.003624 -4.655113

28 6 0 5.477023 -0.081710 -5.526504

29 6 0 4.563641 -1.128447 -5.398586

30 6 0 3.586981 -1.087975 -4.406883

31 6 0 5.477023 -0.081710 5.526504

32 6 0 5.404782 1.003624 4.655113

33 6 0 4.426960 1.041117 3.662366

34 6 0 3.506228 -0.004777 3.521177

35 6 0 3.586981 -1.087975 4.406883

36 6 0 4.563641 -1.128447 5.398586

37 6 0 -3.506229 -0.004755 -3.521190

38 6 0 -3.587078 -1.088005 -4.406825

39 6 0 -4.563750 -1.128466 -5.398519

40 6 0 -5.477043 -0.081661 -5.526509

41 6 0 -5.404706 1.003728 -4.655194

42 6 0 -4.426882 1.041204 -3.662449

43 6 0 -3.506229 -0.004755 3.521190

44 6 0 -3.587078 -1.088005 4.406825

45 6 0 -4.563750 -1.128466 5.398519

46 6 0 -5.477043 -0.081661 5.526509

47 6 0 -5.404706 1.003728 4.655194

48 6 0 -4.426882 1.041204 3.662449

49 1 0 5.117681 -0.229845 1.327571

50 1 0 5.117681 -0.229845 -1.327571

51 1 0 -1.341754 0.374441 -5.098436

52 1 0 1.341822 0.374492 -5.098404

53 1 0 1.341822 0.374492 5.098404

54 1 0 -1.341754 0.374441 5.098436

55 1 0 -5.117653 -0.230096 1.327566

56 1 0 -5.117653 -0.230096 -1.327566

57 1 0 4.370285 1.891877 -2.991779

58 1 0 6.107124 1.825591 -4.749491

59 1 0 6.237826 -0.112174 -6.299581

60 1 0 4.614106 -1.979810 -6.069753

61 1 0 2.881914 -1.906348 -4.309290

62 1 0 6.237826 -0.112174 6.299581

63 1 0 6.107124 1.825591 4.749491

64 1 0 4.370285 1.891877 2.991779

65 1 0 2.881914 -1.906348 4.309290

66 1 0 4.614106 -1.979810 6.069753

67 1 0 -2.882093 -1.906439 -4.309171

68 1 0 -4.614292 -1.979873 -6.069623

69 1 0 -6.237849 -0.112114 -6.299584

70 1 0 -6.106977 1.825750 -4.749629

71 1 0 -4.370127 1.892012 -2.991933

72 1 0 -2.882093 -1.906439 4.309171

73 1 0 -4.614292 -1.979873 6.069623

74 1 0 -6.237849 -0.112114 6.299584

75 1 0 -6.106977 1.825750 4.749629

76 1 0 -4.370127 1.892012 2.991933

77 1 0 1.106428 0.093501 -0.000000

78 1 0 -1.106445 0.093846 0.000000

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

Rotational constants (GHZ): 0.0583459 0.0578412 0.0300209

Leave Link 202 at Sun Aug 18 15:08:17 2019, MaxMem= 2013265920 cpu: 0.1

(Enter /home/kira/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')

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Alpha occ. eigenvalues -- -14.33324 -14.33324 -14.27004 -14.27004 -10.20732

Alpha occ. eigenvalues -- -10.20732 -10.20732 -10.20732 -10.18125 -10.18125

Alpha occ. eigenvalues -- -10.18125 -10.18125 -10.18080 -10.18079 -10.18079

Alpha occ. eigenvalues -- -10.18079 -10.17703 -10.17703 -10.17703 -10.17703

Alpha occ. eigenvalues -- -10.16937 -10.16936 -10.16936 -10.16936 -10.16914

Alpha occ. eigenvalues -- -10.16914 -10.16914 -10.16914 -10.16859 -10.16859

Alpha occ. eigenvalues -- -10.16859 -10.16859 -10.16829 -10.16829 -10.16829

Alpha occ. eigenvalues -- -10.16829 -10.16812 -10.16812 -10.16812 -10.16812

Alpha occ. eigenvalues -- -10.16691 -10.16691 -10.16624 -10.16624 -10.14351

Alpha occ. eigenvalues -- -10.14351 -10.14291 -10.14291 -0.97323 -0.97176

Alpha occ. eigenvalues -- -0.92644 -0.92361 -0.86333 -0.86047 -0.86012

Alpha occ. eigenvalues -- -0.85888 -0.81577 -0.80219 -0.79667 -0.78949

Alpha occ. eigenvalues -- -0.78135 -0.77297 -0.74754 -0.74513 -0.74502

Alpha occ. eigenvalues -- -0.74459 -0.74300 -0.73759 -0.73723 -0.72803

Alpha occ. eigenvalues -- -0.72532 -0.70753 -0.70313 -0.65436 -0.65230

Alpha occ. eigenvalues -- -0.61530 -0.60558 -0.60424 -0.60318 -0.60239

Alpha occ. eigenvalues -- -0.59554 -0.59488 -0.59433 -0.58695 -0.58684

Alpha occ. eigenvalues -- -0.58299 -0.56174 -0.56044 -0.55079 -0.53972

Alpha occ. eigenvalues -- -0.53372 -0.51769 -0.51588 -0.51507 -0.49721

Alpha occ. eigenvalues -- -0.49630 -0.49325 -0.48861 -0.47831 -0.45926

Alpha occ. eigenvalues -- -0.45538 -0.45403 -0.45315 -0.45268 -0.44758

Alpha occ. eigenvalues -- -0.44641 -0.44445 -0.43803 -0.43312 -0.43197

Alpha occ. eigenvalues -- -0.42252 -0.42001 -0.41974 -0.41832 -0.41793

Alpha occ. eigenvalues -- -0.41752 -0.41562 -0.41459 -0.41353 -0.40980

Alpha occ. eigenvalues -- -0.40490 -0.39519 -0.38936 -0.38460 -0.38283

Alpha occ. eigenvalues -- -0.38023 -0.37531 -0.37125 -0.37010 -0.36547

Alpha occ. eigenvalues -- -0.36141 -0.36016 -0.35387 -0.35040 -0.34724

Alpha occ. eigenvalues -- -0.34289 -0.34232 -0.34211 -0.34174 -0.34144

Alpha occ. eigenvalues -- -0.33784 -0.33287 -0.31345 -0.28604 -0.27587

Alpha occ. eigenvalues -- -0.26465 -0.26299 -0.25943 -0.25938 -0.25748

Alpha occ. eigenvalues -- -0.25587 -0.25495 -0.25444 -0.25398 -0.24807

Alpha occ. eigenvalues -- -0.24771 -0.24494 -0.22918 -0.22587 -0.19939

Alpha occ. eigenvalues -- -0.18716 -0.12084

Alpha virt. eigenvalues -- -0.07731 -0.03448 -0.00961 -0.00910 -0.00895

Alpha virt. eigenvalues -- -0.00752 -0.00686 -0.00608 -0.00592 -0.00514

Alpha virt. eigenvalues -- 0.04148 0.05656 0.05830 0.05865 0.05972

Alpha virt. eigenvalues -- 0.06032 0.06529 0.07990 0.08110 0.08635

Alpha virt. eigenvalues -- 0.08695 0.08883 0.09339 0.09665 0.09693

Alpha virt. eigenvalues -- 0.10290 0.10522 0.10542 0.10727 0.10756

Alpha virt. eigenvalues -- 0.11019 0.12025 0.12050 0.12680 0.12839

Alpha virt. eigenvalues -- 0.12940 0.13214 0.13280 0.13627 0.13663

Alpha virt. eigenvalues -- 0.13735 0.13764 0.13976 0.14221 0.14234

Alpha virt. eigenvalues -- 0.14264 0.14464 0.15406 0.15800 0.16366

Alpha virt. eigenvalues -- 0.16714 0.17219 0.18082 0.19975 0.22125

Alpha virt. eigenvalues -- 0.22316 0.23817 0.24047 0.24169 0.24630

Alpha virt. eigenvalues -- 0.24772 0.24922 0.25131 0.25942 0.26137

Alpha virt. eigenvalues -- 0.26754 0.27308 0.27360 0.28059 0.28301

Alpha virt. eigenvalues -- 0.28335 0.28364 0.28677 0.28753 0.29139

Alpha virt. eigenvalues -- 0.29320 0.29396 0.29951 0.29991 0.30246

Alpha virt. eigenvalues -- 0.30429 0.30440 0.31028 0.31429 0.31480

Alpha virt. eigenvalues -- 0.31772 0.32380 0.32492 0.33898 0.34549

Alpha virt. eigenvalues -- 0.35145 0.35638 0.35839 0.36269 0.36328

Alpha virt. eigenvalues -- 0.36471 0.36730 0.36900 0.37201 0.37270

Alpha virt. eigenvalues -- 0.37390 0.38077 0.38146 0.38302 0.38776

Alpha virt. eigenvalues -- 0.39186 0.39399 0.39769 0.40252 0.40406

Alpha virt. eigenvalues -- 0.40419 0.40552 0.40841 0.40878 0.41429

Alpha virt. eigenvalues -- 0.41453 0.41500 0.41505 0.41635 0.41854

Alpha virt. eigenvalues -- 0.42042 0.42243 0.42504 0.42505 0.42563

Alpha virt. eigenvalues -- 0.42900 0.42913 0.43320 0.43360 0.43487

Alpha virt. eigenvalues -- 0.43631 0.43999 0.44269 0.44823 0.44920

Alpha virt. eigenvalues -- 0.45048 0.45181 0.45219 0.45383 0.45534

Alpha virt. eigenvalues -- 0.46122 0.46214 0.46268 0.46529 0.47478

Alpha virt. eigenvalues -- 0.47493 0.47529 0.47624 0.47906 0.47993

Alpha virt. eigenvalues -- 0.48458 0.48991 0.49071 0.49495 0.49726

Alpha virt. eigenvalues -- 0.50320 0.50659 0.51015 0.51669 0.51731

Alpha virt. eigenvalues -- 0.51871 0.52481 0.52666 0.53492 0.53632

Alpha virt. eigenvalues -- 0.53872 0.54200 0.54563 0.54727 0.55511

Alpha virt. eigenvalues -- 0.55902 0.56421 0.57440 0.58057 0.58093

Alpha virt. eigenvalues -- 0.58321 0.58336 0.58416 0.59142 0.59182

Alpha virt. eigenvalues -- 0.59942 0.60305 0.60545 0.60778 0.60913

Alpha virt. eigenvalues -- 0.60944 0.61021 0.61165 0.61414 0.61456

Alpha virt. eigenvalues -- 0.61527 0.61861 0.62132 0.62147 0.62272

Alpha virt. eigenvalues -- 0.62342 0.62927 0.62961 0.63021 0.63273

Alpha virt. eigenvalues -- 0.64279 0.64862 0.65032 0.65057 0.65249

Alpha virt. eigenvalues -- 0.65352 0.65472 0.65666 0.65776 0.65975

Alpha virt. eigenvalues -- 0.66153 0.66235 0.66830 0.67091 0.67629

Alpha virt. eigenvalues -- 0.67681 0.68832 0.69852 0.69959 0.70122

Alpha virt. eigenvalues -- 0.70151 0.70915 0.71207 0.71703 0.72025

Alpha virt. eigenvalues -- 0.72811 0.73051 0.73067 0.73393 0.73557

Alpha virt. eigenvalues -- 0.74155 0.74634 0.74721 0.74863 0.75106

Alpha virt. eigenvalues -- 0.75172 0.75889 0.75957 0.76011 0.76020

Alpha virt. eigenvalues -- 0.76623 0.76637 0.76867 0.77501 0.78458

Alpha virt. eigenvalues -- 0.78772 0.79042 0.79459 0.79670 0.80148

Alpha virt. eigenvalues -- 0.80170 0.80428 0.80743 0.81076 0.81170

Alpha virt. eigenvalues -- 0.81944 0.82351 0.82368 0.82423 0.82851

Alpha virt. eigenvalues -- 0.82943 0.84515 0.85112 0.85472 0.85742

Alpha virt. eigenvalues -- 0.86277 0.86321 0.87552 0.87745 0.87952

Alpha virt. eigenvalues -- 0.88028 0.89640 0.89769 0.89852 0.89984

Alpha virt. eigenvalues -- 0.90002 0.90777 0.91425 0.92578 0.92796

Alpha virt. eigenvalues -- 0.92814 0.93069 0.93682 0.93692 0.95599

Alpha virt. eigenvalues -- 0.96006 0.96162 0.96980 0.97389 0.97663

Alpha virt. eigenvalues -- 0.97896 0.99109 0.99459 1.00408 1.00685

Alpha virt. eigenvalues -- 1.01234 1.01872 1.01885 1.01943 1.03155

Alpha virt. eigenvalues -- 1.03239 1.03313 1.05370 1.05423 1.05784

Alpha virt. eigenvalues -- 1.06516 1.06898 1.08549 1.08710 1.09119

Alpha virt. eigenvalues -- 1.09844 1.10074 1.10545 1.11570 1.12065

Alpha virt. eigenvalues -- 1.12099 1.13864 1.14092 1.14807 1.15070

Alpha virt. eigenvalues -- 1.15392 1.15420 1.16191 1.16251 1.17598

Alpha virt. eigenvalues -- 1.17785 1.17838 1.18025 1.18848 1.19537

Alpha virt. eigenvalues -- 1.20016 1.20490 1.20587 1.20742 1.21340

Alpha virt. eigenvalues -- 1.21690 1.21750 1.21861 1.21967 1.22441

Alpha virt. eigenvalues -- 1.23709 1.23794 1.23941 1.24480 1.25334

Alpha virt. eigenvalues -- 1.25534 1.25622 1.25844 1.25929 1.26323

Alpha virt. eigenvalues -- 1.26702 1.26760 1.26797 1.27908 1.28887

Alpha virt. eigenvalues -- 1.29082 1.29649 1.30523 1.31941 1.32042

Alpha virt. eigenvalues -- 1.32351 1.32436 1.33691 1.34411 1.38115

Alpha virt. eigenvalues -- 1.38901 1.39542 1.41231 1.41337 1.41746

Alpha virt. eigenvalues -- 1.41858 1.42855 1.42980 1.42995 1.44710

Alpha virt. eigenvalues -- 1.45710 1.46083 1.46342 1.47877 1.48025

Alpha virt. eigenvalues -- 1.48166 1.48185 1.48691 1.48968 1.49372

Alpha virt. eigenvalues -- 1.49582 1.49679 1.49855 1.50230 1.50455

Alpha virt. eigenvalues -- 1.52287 1.53708 1.54117 1.54226 1.54736

Alpha virt. eigenvalues -- 1.54762 1.55084 1.55964 1.57321 1.58551

Alpha virt. eigenvalues -- 1.59087 1.59971 1.62258 1.62557 1.63058

Alpha virt. eigenvalues -- 1.63250 1.63373 1.65073 1.65987 1.66503

Alpha virt. eigenvalues -- 1.68194 1.68583 1.68751 1.69354 1.69624

Alpha virt. eigenvalues -- 1.70598 1.70958 1.71451 1.71630 1.72284

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Alpha virt. eigenvalues -- 1.93010 1.93168 1.93169 1.93765 1.94086

Alpha virt. eigenvalues -- 1.94486 1.94620 1.94742 1.95162 1.95241

Alpha virt. eigenvalues -- 1.95380 1.96605 1.96825 1.97121 1.97212

Alpha virt. eigenvalues -- 1.97307 1.98029 1.98707 1.99157 2.00253

Alpha virt. eigenvalues -- 2.00709 2.01006 2.01152 2.01261 2.03999

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Alpha virt. eigenvalues -- 2.09338 2.09883 2.11301 2.13582 2.14590

Alpha virt. eigenvalues -- 2.14872 2.18529 2.19828 2.22687 2.24306

Alpha virt. eigenvalues -- 2.24464 2.24494 2.25938 2.26106 2.26527

Alpha virt. eigenvalues -- 2.26933 2.27102 2.27442 2.27573 2.27606

Alpha virt. eigenvalues -- 2.28052 2.28496 2.28605 2.28640 2.28836

Alpha virt. eigenvalues -- 2.28933 2.29871 2.29989 2.30224 2.30633

Alpha virt. eigenvalues -- 2.31968 2.32233 2.32944 2.33112 2.33135

Alpha virt. eigenvalues -- 2.33976 2.34184 2.34760 2.36108 2.36278

Alpha virt. eigenvalues -- 2.36328 2.36549 2.36948 2.37755 2.37861

Alpha virt. eigenvalues -- 2.38772 2.39810 2.40079 2.40415 2.41778

Alpha virt. eigenvalues -- 2.42020 2.42307 2.44222 2.44729 2.45818

Alpha virt. eigenvalues -- 2.47953 2.48588 2.49588 2.50684 2.53410

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Alpha virt. eigenvalues -- 2.56720 2.58033 2.58158 2.58688 2.59331

Alpha virt. eigenvalues -- 2.59970 2.59981 2.60750 2.61650 2.62442

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Alpha virt. eigenvalues -- 4.00058 4.00089 4.05234 4.12711 4.30425

Alpha virt. eigenvalues -- 4.31958 4.37622 4.41470 4.47309 4.52372

Alpha virt. eigenvalues -- 4.56457 4.58301 4.65569 4.65977 4.69383

Alpha virt. eigenvalues -- 4.71327 4.79173 4.79182 4.79190 4.79199

Alpha virt. eigenvalues -- 5.10707 5.16737 5.19592 5.31715 23.25606

Alpha virt. eigenvalues -- 23.29141 23.29344 23.30965 23.46604 23.52842

Alpha virt. eigenvalues -- 23.55136 23.60430 23.74999 23.77755 23.77770

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Alpha virt. eigenvalues -- 24.01768 24.02111 24.05102 24.05225 24.05284

Alpha virt. eigenvalues -- 24.05418 24.10563 24.10689 24.11951 24.12017

Alpha virt. eigenvalues -- 24.13573 24.13651 24.14366 24.14804 24.17677

Alpha virt. eigenvalues -- 24.17718 24.17878 24.18026 35.57248 35.58178

Alpha virt. eigenvalues -- 35.65010 35.65631

Beta occ. eigenvalues -- -14.33167 -14.33167 -14.27060 -14.27060 -10.20712

Beta occ. eigenvalues -- -10.20712 -10.20712 -10.20712 -10.18089 -10.18089

Beta occ. eigenvalues -- -10.18089 -10.18088 -10.18003 -10.18003 -10.18003

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Beta occ. eigenvalues -- -10.16935 -10.16935 -10.16935 -10.16935 -10.16913

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Beta occ. eigenvalues -- -10.16853 -10.16853 -10.16820 -10.16820 -10.16820

Beta occ. eigenvalues -- -10.16820 -10.16806 -10.16806 -10.16806 -10.16806

Beta occ. eigenvalues -- -10.16687 -10.16687 -10.16620 -10.16620 -10.14257

Beta occ. eigenvalues -- -10.14257 -10.14196 -10.14196 -0.97127 -0.96979

Beta occ. eigenvalues -- -0.92479 -0.92197 -0.86272 -0.86008 -0.85976

Beta occ. eigenvalues -- -0.85861 -0.81376 -0.80032 -0.79464 -0.78804

Beta occ. eigenvalues -- -0.78026 -0.77202 -0.74672 -0.74496 -0.74478

Beta occ. eigenvalues -- -0.74445 -0.74233 -0.73678 -0.73567 -0.72699

Beta occ. eigenvalues -- -0.72402 -0.70501 -0.70155 -0.65175 -0.65049

Beta occ. eigenvalues -- -0.61448 -0.60525 -0.60406 -0.60293 -0.60216

Beta occ. eigenvalues -- -0.59473 -0.59425 -0.59410 -0.58655 -0.58532

Beta occ. eigenvalues -- -0.58193 -0.56033 -0.56010 -0.54995 -0.53836

Beta occ. eigenvalues -- -0.53242 -0.51688 -0.51570 -0.51417 -0.49620

Beta occ. eigenvalues -- -0.49574 -0.49229 -0.48764 -0.47772 -0.45897

Beta occ. eigenvalues -- -0.45485 -0.45297 -0.45241 -0.45217 -0.44716

Beta occ. eigenvalues -- -0.44604 -0.44388 -0.43771 -0.43277 -0.43113

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Beta occ. eigenvalues -- -0.34220 -0.34200 -0.34184 -0.34154 -0.34109

Beta occ. eigenvalues -- -0.33743 -0.33241 -0.30688 -0.27950 -0.27015

Beta occ. eigenvalues -- -0.26123 -0.25941 -0.25857 -0.25849 -0.25659

Beta occ. eigenvalues -- -0.25550 -0.25468 -0.25372 -0.25311 -0.24749

Beta occ. eigenvalues -- -0.24659 -0.24068 -0.22466 -0.22268 -0.18792

Beta occ. eigenvalues -- -0.17679

Beta virt. eigenvalues -- -0.08215 -0.07572 -0.02432 -0.00915 -0.00874

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Beta virt. eigenvalues -- 0.06041 0.06763 0.06823 0.08133 0.08480

Beta virt. eigenvalues -- 0.08657 0.08709 0.08901 0.09353 0.09684

Beta virt. eigenvalues -- 0.09710 0.10306 0.10537 0.10561 0.10739

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Beta virt. eigenvalues -- 0.12957 0.12986 0.13271 0.13287 0.13653

Beta virt. eigenvalues -- 0.13829 0.13861 0.13917 0.13986 0.14267

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Beta virt. eigenvalues -- 0.61465 0.61542 0.61887 0.62161 0.62265

Beta virt. eigenvalues -- 0.62336 0.62446 0.62982 0.63043 0.63095

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Beta virt. eigenvalues -- 0.65321 0.65407 0.65511 0.65701 0.65838

Beta virt. eigenvalues -- 0.66012 0.66173 0.66291 0.66882 0.67109

Beta virt. eigenvalues -- 0.67731 0.67792 0.68909 0.70000 0.70002

Beta virt. eigenvalues -- 0.70176 0.70280 0.70951 0.71268 0.71801

Beta virt. eigenvalues -- 0.72155 0.72870 0.73157 0.73165 0.73454

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Beta virt. eigenvalues -- 3.41974 3.42662 3.43237 3.45608 3.46431

Beta virt. eigenvalues -- 3.50910 3.52262 3.52320 3.53122 3.57006

Beta virt. eigenvalues -- 3.57198 3.58292 3.58495 3.58639 3.60052

Beta virt. eigenvalues -- 3.62901 3.63884 3.64156 3.66678 3.66963

Beta virt. eigenvalues -- 3.68023 3.72893 3.73079 3.74061 3.76619

Beta virt. eigenvalues -- 3.78760 3.79290 3.82876 3.82899 3.83396

Beta virt. eigenvalues -- 3.84518 3.88422 3.90599 3.92889 3.95485

Beta virt. eigenvalues -- 3.95884 3.96005 3.96278 3.96403 3.96669

Beta virt. eigenvalues -- 3.96696 4.00155 4.00194 4.05351 4.12819

Beta virt. eigenvalues -- 4.30522 4.32104 4.37737 4.41608 4.47466

Beta virt. eigenvalues -- 4.52450 4.56700 4.58389 4.65692 4.66125

Beta virt. eigenvalues -- 4.69583 4.71512 4.79181 4.79190 4.79199

Beta virt. eigenvalues -- 4.79207 5.10825 5.16864 5.19697 5.31836

Beta virt. eigenvalues -- 23.25618 23.29148 23.29350 23.30969 23.46658

Beta virt. eigenvalues -- 23.52865 23.55248 23.60502 23.75088 23.77834

Beta virt. eigenvalues -- 23.77853 23.80524 23.81396 23.81536 23.81538

Beta virt. eigenvalues -- 23.81776 23.85637 23.86518 23.86535 23.87246

Beta virt. eigenvalues -- 23.92603 23.93200 23.96453 23.97553 24.00645

Beta virt. eigenvalues -- 24.00987 24.01791 24.02129 24.05107 24.05230

Beta virt. eigenvalues -- 24.05290 24.05424 24.10603 24.10727 24.11986

Beta virt. eigenvalues -- 24.12054 24.13653 24.13758 24.14374 24.14838

Beta virt. eigenvalues -- 24.17707 24.17747 24.17914 24.18061 35.57410

Beta virt. eigenvalues -- 35.58340 35.64953 35.65574

Condensed to atoms (all electrons):

Atomic-Atomic Spin Densities.

Mulliken charges and spin densities:

1 2

1 C -0.272818 0.003924

2 C 0.336133 0.015651

3 N -0.730291 0.066943

4 C 0.336133 0.015651

5 C -0.272818 0.003924

6 C -0.138629 0.066176

7 C 0.181929 0.080444

8 N -0.505220 -0.029171

9 C 0.181924 0.080443

10 C -0.297725 0.065371

11 C -0.297722 0.065371

12 C -0.138629 0.066176

13 C 0.181929 0.080444

14 C -0.297722 0.065371

15 C -0.297725 0.065371

16 C 0.181924 0.080443

17 N -0.505220 -0.029171

18 C -0.138638 0.066180

19 C 0.336150 0.015650

20 C -0.272822 0.003923

21 C -0.272822 0.003923

22 C 0.336150 0.015650

23 N -0.730293 0.066945

24 C -0.138638 0.066180

25 C -0.105014 -0.006733

26 C -0.219525 0.007375

27 C -0.220091 -0.001229

28 C -0.226536 0.004239

29 C -0.221644 -0.000080

30 C -0.212045 0.002374

31 C -0.226536 0.004239

32 C -0.220091 -0.001229

33 C -0.219525 0.007375

34 C -0.105014 -0.006733

35 C -0.212045 0.002374

36 C -0.221644 -0.000080

37 C -0.105027 -0.006732

38 C -0.212039 0.002373

39 C -0.221645 -0.000079

40 C -0.226536 0.004237

41 C -0.220093 -0.001229

42 C -0.219507 0.007374

43 C -0.105027 -0.006732

44 C -0.212039 0.002373

45 C -0.221645 -0.000079

46 C -0.226536 0.004237

47 C -0.220093 -0.001229

48 C -0.219507 0.007374

49 H 0.240227 -0.000067

50 H 0.240227 -0.000067

51 H 0.214002 -0.004151

52 H 0.214006 -0.004151

53 H 0.214006 -0.004151

54 H 0.214002 -0.004151

55 H 0.240222 -0.000067

56 H 0.240222 -0.000067

57 H 0.219590 -0.000637

58 H 0.223123 0.000099

59 H 0.222900 -0.000240

60 H 0.223096 0.000156

61 H 0.217938 -0.000245

62 H 0.222900 -0.000240

63 H 0.223123 0.000099

64 H 0.219590 -0.000637

65 H 0.217938 -0.000245

66 H 0.223096 0.000156

67 H 0.217935 -0.000244

68 H 0.223096 0.000156

69 H 0.222901 -0.000240

70 H 0.223123 0.000099

71 H 0.219584 -0.000637

72 H 0.217935 -0.000244

73 H 0.223096 0.000156

74 H 0.222901 -0.000240

75 H 0.223123 0.000099

76 H 0.219584 -0.000637

77 H 0.405687 -0.002625

78 H 0.405690 -0.002626

Sum of Mulliken charges = -1.00000 1.00000

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

1 2

1 C -0.032591 0.003856

2 C 0.336133 0.015651

3 N -0.324604 0.064318

4 C 0.336133 0.015651

5 C -0.032591 0.003856

6 C -0.138629 0.066176

7 C 0.181929 0.080444

8 N -0.505220 -0.029171

9 C 0.181924 0.080443

10 C -0.083723 0.061220

11 C -0.083716 0.061220

12 C -0.138629 0.066176

13 C 0.181929 0.080444

14 C -0.083716 0.061220

15 C -0.083723 0.061220

16 C 0.181924 0.080443

17 N -0.505220 -0.029171

18 C -0.138638 0.066180

19 C 0.336150 0.015650

20 C -0.032600 0.003856

21 C -0.032600 0.003856

22 C 0.336150 0.015650

23 N -0.324603 0.064319

24 C -0.138638 0.066180

25 C -0.105014 -0.006733

26 C 0.000065 0.006738

27 C 0.003032 -0.001130

28 C -0.003636 0.003999

29 C 0.001452 0.000076

30 C 0.005892 0.002129

31 C -0.003636 0.003999

32 C 0.003032 -0.001130

33 C 0.000065 0.006738

34 C -0.105014 -0.006733

35 C 0.005892 0.002129

36 C 0.001452 0.000076

37 C -0.105027 -0.006732

38 C 0.005897 0.002128

39 C 0.001451 0.000077

40 C -0.003635 0.003997

41 C 0.003031 -0.001129

42 C 0.000077 0.006737

43 C -0.105027 -0.006732

44 C 0.005897 0.002128

45 C 0.001451 0.000077

46 C -0.003635 0.003997

47 C 0.003031 -0.001129

48 C 0.000077 0.006737

Electronic spatial extent (au): <R\*\*2>= 33462.1369

Charge= -1.0000 electrons

Dipole moment (field-independent basis, Debye):

X= -0.0000 Y= -0.2677 Z= -0.0000 Tot= 0.2677

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

XX= -259.2468 YY= -275.0381 ZZ= -291.8932

XY= 0.0017 XZ= 0.0000 YZ= -0.0000

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

XX= 16.1459 YY= 0.3546 ZZ= -16.5005

XY= 0.0017 XZ= 0.0000 YZ= -0.0000

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

XXX= 0.0120 YYY= -4.3506 ZZZ= 0.0000 XYY= -0.0094

XXY= 85.4733 XXZ= 0.0000 XZZ= -0.0074 YZZ= -95.4135

YYZ= -0.0000 XYZ= 0.0000

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

XXXX= -21908.8489 YYYY= -1090.6302 ZZZZ= -22864.3520 XXXY= 0.1002

XXXZ= 0.0000 YYYX= -0.0021 YYYZ= 0.0000 ZZZX= -0.0000

ZZZY= 0.0000 XXYY= -3880.2242 XXZZ= -6244.0624 YYZZ= -3918.3868

XXYZ= -0.0000 YYXZ= -0.0000 ZZXY= -0.0128

N-N= 5.345867316649D+03 E-N=-1.517667742509D+04 KE= 1.906564245666D+03

Symmetry A' KE= 1.008388339568D+03

Symmetry A" KE= 8.981759060979D+02

Isotropic Fermi Contact Couplings

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

1 C(13) -0.00064 -0.71535 -0.25526 -0.23862

2 C(13) -0.00364 -4.08667 -1.45822 -1.36317

3 N(14) 0.00874 2.82364 1.00754 0.94186

4 C(13) -0.00364 -4.08667 -1.45822 -1.36317

5 C(13) -0.00064 -0.71535 -0.25526 -0.23862

6 C(13) 0.00150 1.68452 0.60108 0.56189

7 C(13) 0.00189 2.12197 0.75717 0.70781

8 N(14) -0.00521 -1.68372 -0.60079 -0.56163

9 C(13) 0.00189 2.12186 0.75713 0.70778

10 C(13) -0.00010 -0.10831 -0.03865 -0.03613

11 C(13) -0.00010 -0.10830 -0.03864 -0.03612

12 C(13) 0.00150 1.68452 0.60108 0.56189

13 C(13) 0.00189 2.12197 0.75717 0.70781

14 C(13) -0.00010 -0.10830 -0.03864 -0.03612

15 C(13) -0.00010 -0.10831 -0.03865 -0.03613

16 C(13) 0.00189 2.12186 0.75713 0.70778

17 N(14) -0.00521 -1.68372 -0.60079 -0.56163

18 C(13) 0.00150 1.68506 0.60127 0.56208

19 C(13) -0.00364 -4.08758 -1.45855 -1.36347

20 C(13) -0.00064 -0.71543 -0.25528 -0.23864

21 C(13) -0.00064 -0.71543 -0.25528 -0.23864

22 C(13) -0.00364 -4.08758 -1.45855 -1.36347

23 N(14) 0.00874 2.82329 1.00742 0.94175

24 C(13) 0.00150 1.68506 0.60127 0.56208

25 C(13) -0.00277 -3.11607 -1.11189 -1.03941

26 C(13) 0.00276 3.10278 1.10715 1.03498

27 C(13) 0.00019 0.21425 0.07645 0.07147

28 C(13) 0.00027 0.30307 0.10814 0.10109

29 C(13) -0.00013 -0.14905 -0.05319 -0.04972

30 C(13) 0.00093 1.04852 0.37414 0.34975

31 C(13) 0.00027 0.30307 0.10814 0.10109

32 C(13) 0.00019 0.21425 0.07645 0.07147

33 C(13) 0.00276 3.10278 1.10715 1.03498

34 C(13) -0.00277 -3.11607 -1.11189 -1.03941

35 C(13) 0.00093 1.04852 0.37414 0.34975

36 C(13) -0.00013 -0.14905 -0.05319 -0.04972

37 C(13) -0.00277 -3.11615 -1.11192 -1.03944

38 C(13) 0.00093 1.04916 0.37437 0.34996

39 C(13) -0.00013 -0.14885 -0.05311 -0.04965

40 C(13) 0.00027 0.30297 0.10811 0.10106

41 C(13) 0.00019 0.21445 0.07652 0.07153

42 C(13) 0.00276 3.10322 1.10731 1.03512

43 C(13) -0.00277 -3.11615 -1.11192 -1.03944

44 C(13) 0.00093 1.04916 0.37437 0.34996

45 C(13) -0.00013 -0.14885 -0.05311 -0.04965

46 C(13) 0.00027 0.30297 0.10811 0.10106

47 C(13) 0.00019 0.21445 0.07652 0.07153

48 C(13) 0.00276 3.10322 1.10731 1.03512

49 H(1) -0.00007 -0.30450 -0.10865 -0.10157

50 H(1) -0.00007 -0.30450 -0.10865 -0.10157

51 H(1) -0.00120 -5.37215 -1.91692 -1.79196

52 H(1) -0.00120 -5.37206 -1.91688 -1.79193

53 H(1) -0.00120 -5.37206 -1.91688 -1.79193

54 H(1) -0.00120 -5.37215 -1.91692 -1.79196

55 H(1) -0.00007 -0.30441 -0.10862 -0.10154

56 H(1) -0.00007 -0.30441 -0.10862 -0.10154

57 H(1) -0.00009 -0.42262 -0.15080 -0.14097

58 H(1) 0.00003 0.13077 0.04666 0.04362

59 H(1) -0.00006 -0.26561 -0.09478 -0.08860

60 H(1) 0.00006 0.26971 0.09624 0.08996

61 H(1) -0.00003 -0.11788 -0.04206 -0.03932

62 H(1) -0.00006 -0.26561 -0.09478 -0.08860

63 H(1) 0.00003 0.13077 0.04666 0.04362

64 H(1) -0.00009 -0.42262 -0.15080 -0.14097

65 H(1) -0.00003 -0.11788 -0.04206 -0.03932

66 H(1) 0.00006 0.26971 0.09624 0.08996

67 H(1) -0.00003 -0.11795 -0.04209 -0.03934

68 H(1) 0.00006 0.26971 0.09624 0.08996

69 H(1) -0.00006 -0.26552 -0.09474 -0.08857

70 H(1) 0.00003 0.13077 0.04666 0.04362

71 H(1) -0.00009 -0.42254 -0.15077 -0.14094

72 H(1) -0.00003 -0.11795 -0.04209 -0.03934

73 H(1) 0.00006 0.26971 0.09624 0.08996

74 H(1) -0.00006 -0.26552 -0.09474 -0.08857

75 H(1) 0.00003 0.13077 0.04666 0.04362

76 H(1) -0.00009 -0.42254 -0.15077 -0.14094

77 H(1) -0.00120 -5.36741 -1.91522 -1.79037

78 H(1) -0.00120 -5.36877 -1.91571 -1.79083

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

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

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1 Atom -0.001174 0.003067 -0.001893

2 Atom -0.016304 0.024084 -0.007780

3 Atom -0.090101 0.176616 -0.086516

4 Atom -0.016304 0.024084 -0.007780

5 Atom -0.001174 0.003067 -0.001893

6 Atom -0.047903 0.095813 -0.047910

7 Atom -0.052543 0.103234 -0.050691

8 Atom 0.027113 -0.052036 0.024923

9 Atom -0.052542 0.103235 -0.050693

10 Atom -0.042439 0.080834 -0.038395

11 Atom -0.042439 0.080833 -0.038394

12 Atom -0.047903 0.095813 -0.047910

13 Atom -0.052543 0.103234 -0.050691

14 Atom -0.042439 0.080833 -0.038394

15 Atom -0.042439 0.080834 -0.038395

16 Atom -0.052542 0.103235 -0.050693

17 Atom 0.027113 -0.052036 0.024923

18 Atom -0.047906 0.095817 -0.047912

19 Atom -0.016302 0.024081 -0.007779

20 Atom -0.001173 0.003065 -0.001893

21 Atom -0.001173 0.003065 -0.001893

22 Atom -0.016302 0.024081 -0.007779

23 Atom -0.090094 0.176612 -0.086518

24 Atom -0.047906 0.095817 -0.047912

25 Atom 0.000691 -0.001496 0.000804

26 Atom 0.006262 -0.004068 -0.002194

27 Atom 0.001619 -0.000768 -0.000851

28 Atom 0.000217 -0.000961 0.000744

29 Atom 0.001054 -0.000270 -0.000784

30 Atom 0.000291 -0.002764 0.002473

31 Atom 0.000217 -0.000961 0.000744

32 Atom 0.001619 -0.000768 -0.000851

33 Atom 0.006262 -0.004068 -0.002194

34 Atom 0.000691 -0.001496 0.000804

35 Atom 0.000291 -0.002764 0.002473

36 Atom 0.001054 -0.000270 -0.000784

37 Atom 0.000691 -0.001495 0.000804

38 Atom 0.000290 -0.002762 0.002472

39 Atom 0.001054 -0.000270 -0.000785

40 Atom 0.000217 -0.000961 0.000744

41 Atom 0.001619 -0.000768 -0.000851

42 Atom 0.006262 -0.004068 -0.002194

43 Atom 0.000691 -0.001495 0.000804

44 Atom 0.000290 -0.002762 0.002472

45 Atom 0.001054 -0.000270 -0.000785

46 Atom 0.000217 -0.000961 0.000744

47 Atom 0.001619 -0.000768 -0.000851

48 Atom 0.006262 -0.004068 -0.002194

49 Atom 0.001230 -0.001393 0.000163

50 Atom 0.001230 -0.001393 0.000163

51 Atom -0.002696 -0.001946 0.004642

52 Atom -0.002695 -0.001946 0.004642

53 Atom -0.002695 -0.001946 0.004642

54 Atom -0.002696 -0.001946 0.004642

55 Atom 0.001230 -0.001393 0.000163

56 Atom 0.001230 -0.001393 0.000163

57 Atom 0.000639 -0.000305 -0.000334

58 Atom 0.000366 -0.000232 -0.000134

59 Atom 0.000316 -0.000530 0.000214

60 Atom 0.000130 -0.000297 0.000167

61 Atom 0.000093 0.000054 -0.000147

62 Atom 0.000316 -0.000530 0.000214

63 Atom 0.000366 -0.000232 -0.000134

64 Atom 0.000639 -0.000305 -0.000334

65 Atom 0.000093 0.000054 -0.000147

66 Atom 0.000130 -0.000297 0.000167

67 Atom 0.000093 0.000054 -0.000147

68 Atom 0.000130 -0.000297 0.000167

69 Atom 0.000316 -0.000530 0.000214

70 Atom 0.000366 -0.000232 -0.000134

71 Atom 0.000638 -0.000305 -0.000334

72 Atom 0.000093 0.000054 -0.000147

73 Atom 0.000130 -0.000297 0.000167

74 Atom 0.000316 -0.000530 0.000214

75 Atom 0.000366 -0.000232 -0.000134

76 Atom 0.000638 -0.000305 -0.000334

77 Atom 0.009243 -0.004274 -0.004969

78 Atom 0.009243 -0.004273 -0.004970

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XY XZ YZ

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1 Atom 0.000179 -0.000526 0.000647

2 Atom 0.002147 -0.000151 0.001589

3 Atom 0.019916 0.000000 0.000000

4 Atom 0.002147 0.000151 -0.001589

5 Atom 0.000179 0.000526 -0.000647

6 Atom 0.008026 0.002537 0.000146

7 Atom 0.001973 0.003837 0.014925

8 Atom -0.000001 0.000000 -0.008090

9 Atom -0.001970 -0.003836 0.014916

10 Atom 0.000202 0.000372 0.021214

11 Atom -0.000208 -0.000374 0.021218

12 Atom 0.008026 -0.002537 -0.000146

13 Atom 0.001973 -0.003837 -0.014925

14 Atom -0.000208 0.000374 -0.021218

15 Atom 0.000202 -0.000372 -0.021214

16 Atom -0.001970 0.003836 -0.014916

17 Atom -0.000001 -0.000000 0.008090

18 Atom -0.008023 0.002536 -0.000145

19 Atom -0.002155 0.000150 0.001589

20 Atom -0.000181 0.000526 0.000645

21 Atom -0.000181 -0.000526 -0.000645

22 Atom -0.002155 -0.000150 -0.001589

23 Atom -0.019978 -0.000000 0.000000

24 Atom -0.008023 -0.002536 0.000145

25 Atom 0.001507 -0.002946 0.001375

26 Atom -0.001173 0.002220 -0.001319

27 Atom 0.000251 -0.001485 0.000696

28 Atom -0.002094 0.001965 -0.002391

29 Atom -0.000796 -0.000813 0.000369

30 Atom 0.000026 0.001916 0.002925

31 Atom -0.002094 -0.001965 0.002391

32 Atom 0.000251 0.001485 -0.000696

33 Atom -0.001173 -0.002220 0.001319

34 Atom 0.001507 0.002946 -0.001375

35 Atom 0.000026 -0.001916 -0.002925

36 Atom -0.000796 0.000813 -0.000369

37 Atom -0.001507 0.002946 0.001375

38 Atom -0.000026 -0.001914 0.002926

39 Atom 0.000797 0.000813 0.000369

40 Atom 0.002092 -0.001964 -0.002390

41 Atom -0.000251 0.001485 0.000695

42 Atom 0.001171 -0.002219 -0.001318

43 Atom -0.001507 -0.002946 -0.001375

44 Atom -0.000026 0.001914 -0.002926

45 Atom 0.000797 -0.000813 -0.000369

46 Atom 0.002092 0.001964 0.002390

47 Atom -0.000251 -0.001485 -0.000695

48 Atom 0.001171 0.002219 0.001318

49 Atom -0.000293 0.000268 -0.000023

50 Atom -0.000293 -0.000268 0.000023

51 Atom -0.001036 0.005875 -0.001021

52 Atom 0.001036 -0.005875 -0.001022

53 Atom 0.001036 0.005875 0.001022

54 Atom -0.001036 -0.005875 0.001021

55 Atom 0.000293 -0.000268 -0.000023

56 Atom 0.000293 0.000268 0.000023

57 Atom 0.001593 -0.000475 -0.000165

58 Atom 0.000274 -0.000428 -0.000092

59 Atom -0.000151 -0.000581 -0.000007

60 Atom -0.000302 -0.000488 0.000374

61 Atom -0.001159 -0.000814 0.001143

62 Atom -0.000151 0.000581 0.000007

63 Atom 0.000274 0.000428 0.000092

64 Atom 0.001593 0.000475 0.000165

65 Atom -0.001159 0.000814 -0.001143

66 Atom -0.000302 0.000488 -0.000374

67 Atom 0.001159 0.000814 0.001143

68 Atom 0.000302 0.000488 0.000374

69 Atom 0.000151 0.000581 -0.000007

70 Atom -0.000274 0.000428 -0.000092

71 Atom -0.001593 0.000476 -0.000165

72 Atom 0.001159 -0.000814 -0.001143

73 Atom 0.000302 -0.000488 -0.000374

74 Atom 0.000151 -0.000581 0.000007

75 Atom -0.000274 -0.000428 0.000092

76 Atom -0.001593 -0.000476 0.000165

77 Atom -0.000647 -0.000000 0.000000

78 Atom 0.000651 -0.000000 0.000000

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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 -0.0023 -0.302 -0.108 -0.101 0.4514 -0.1227 0.8838

1 C(13) Bbb -0.0009 -0.121 -0.043 -0.040 0.8919 0.0334 -0.4509

Bcc 0.0032 0.423 0.151 0.141 0.0258 0.9919 0.1245

Baa -0.0164 -2.204 -0.786 -0.735 0.9982 -0.0540 0.0273

2 C(13) Bbb -0.0079 -1.054 -0.376 -0.351 -0.0299 -0.0477 0.9984

Bcc 0.0243 3.258 1.162 1.087 0.0526 0.9974 0.0492

Baa -0.0916 -3.532 -1.260 -1.178 0.9973 -0.0741 -0.0000

3 N(14) Bbb -0.0865 -3.337 -1.191 -1.113 0.0000 -0.0000 1.0000

Bcc 0.1781 6.869 2.451 2.291 0.0741 0.9973 0.0000

Baa -0.0164 -2.204 -0.786 -0.735 0.9982 -0.0540 -0.0273

4 C(13) Bbb -0.0079 -1.054 -0.376 -0.351 0.0299 0.0477 0.9984

Bcc 0.0243 3.258 1.162 1.087 0.0526 0.9974 -0.0492

Baa -0.0023 -0.302 -0.108 -0.101 -0.4514 0.1227 0.8838

5 C(13) Bbb -0.0009 -0.121 -0.043 -0.040 0.8919 0.0334 0.4509

Bcc 0.0032 0.423 0.151 0.141 0.0258 0.9919 -0.1245

Baa -0.0507 -6.799 -2.426 -2.268 0.7361 -0.0397 -0.6757

6 C(13) Bbb -0.0456 -6.119 -2.183 -2.041 0.6746 -0.0390 0.7372

Bcc 0.0963 12.917 4.609 4.309 0.0556 0.9985 0.0020

Baa -0.0560 -7.513 -2.681 -2.506 0.7287 0.0550 -0.6826

7 C(13) Bbb -0.0487 -6.537 -2.333 -2.180 0.6847 -0.0800 0.7244

Bcc 0.1047 14.050 5.013 4.687 0.0148 0.9953 0.0960

Baa -0.0529 -2.039 -0.728 -0.680 0.0000 0.9946 0.1034

8 N(14) Bbb 0.0258 0.994 0.355 0.331 -0.0002 -0.1034 0.9946

Bcc 0.0271 1.046 0.373 0.349 1.0000 -0.0000 0.0002

Baa -0.0560 -7.513 -2.681 -2.506 0.7287 -0.0549 0.6827

9 C(13) Bbb -0.0487 -6.537 -2.333 -2.180 -0.6847 -0.0800 0.7244

Bcc 0.1047 14.050 5.013 4.687 -0.0148 0.9953 0.0959

Baa -0.0426 -5.721 -2.041 -1.908 0.8656 0.0834 -0.4937

10 C(13) Bbb -0.0419 -5.618 -2.005 -1.874 0.5007 -0.1483 0.8528

Bcc 0.0845 11.339 4.046 3.782 0.0021 0.9854 0.1701

Baa -0.0426 -5.721 -2.041 -1.908 0.8657 -0.0834 0.4936

11 C(13) Bbb -0.0419 -5.618 -2.005 -1.874 -0.5006 -0.1483 0.8529

Bcc 0.0845 11.339 4.046 3.782 -0.0021 0.9854 0.1701

Baa -0.0507 -6.799 -2.426 -2.268 0.7361 -0.0397 0.6757

12 C(13) Bbb -0.0456 -6.119 -2.183 -2.041 -0.6746 0.0390 0.7372

Bcc 0.0963 12.917 4.609 4.309 0.0556 0.9985 -0.0020

Baa -0.0560 -7.513 -2.681 -2.506 0.7287 0.0550 0.6826

13 C(13) Bbb -0.0487 -6.537 -2.333 -2.180 -0.6847 0.0800 0.7244

Bcc 0.1047 14.050 5.013 4.687 0.0148 0.9953 -0.0960

Baa -0.0426 -5.721 -2.041 -1.908 0.8657 -0.0834 -0.4936

14 C(13) Bbb -0.0419 -5.618 -2.005 -1.874 0.5006 0.1483 0.8529

Bcc 0.0845 11.339 4.046 3.782 -0.0021 0.9854 -0.1701

Baa -0.0426 -5.721 -2.041 -1.908 0.8656 0.0834 0.4937

15 C(13) Bbb -0.0419 -5.618 -2.005 -1.874 -0.5007 0.1483 0.8528

Bcc 0.0845 11.339 4.046 3.782 0.0021 0.9854 -0.1701

Baa -0.0560 -7.513 -2.681 -2.506 0.7287 -0.0549 -0.6827

16 C(13) Bbb -0.0487 -6.537 -2.333 -2.180 0.6847 0.0800 0.7244

Bcc 0.1047 14.050 5.013 4.687 -0.0148 0.9953 -0.0959

Baa -0.0529 -2.039 -0.728 -0.680 0.0000 0.9946 -0.1034

17 N(14) Bbb 0.0258 0.994 0.355 0.331 0.0002 0.1034 0.9946

Bcc 0.0271 1.046 0.373 0.349 1.0000 -0.0000 -0.0002

Baa -0.0507 -6.799 -2.426 -2.268 0.7361 0.0396 -0.6757

18 C(13) Bbb -0.0456 -6.119 -2.183 -2.041 0.6746 0.0390 0.7371

Bcc 0.0963 12.918 4.609 4.309 -0.0556 0.9985 -0.0020

Baa -0.0164 -2.204 -0.786 -0.735 0.9982 0.0542 -0.0273

19 C(13) Bbb -0.0079 -1.053 -0.376 -0.351 0.0299 -0.0477 0.9984

Bcc 0.0243 3.257 1.162 1.086 -0.0528 0.9974 0.0492

Baa -0.0023 -0.302 -0.108 -0.101 -0.4516 -0.1226 0.8838

20 C(13) Bbb -0.0009 -0.121 -0.043 -0.040 0.8918 -0.0326 0.4512

Bcc 0.0032 0.423 0.151 0.141 -0.0265 0.9919 0.1241

Baa -0.0023 -0.302 -0.108 -0.101 0.4516 0.1226 0.8838

21 C(13) Bbb -0.0009 -0.121 -0.043 -0.040 0.8918 -0.0326 -0.4512

Bcc 0.0032 0.423 0.151 0.141 -0.0265 0.9919 -0.1241

Baa -0.0164 -2.204 -0.786 -0.735 0.9982 0.0542 0.0273

22 C(13) Bbb -0.0079 -1.053 -0.376 -0.351 -0.0299 0.0477 0.9984

Bcc 0.0243 3.257 1.162 1.086 -0.0528 0.9974 -0.0492

Baa -0.0916 -3.532 -1.260 -1.178 0.9972 0.0743 0.0000

23 N(14) Bbb -0.0865 -3.337 -1.191 -1.113 -0.0000 -0.0000 1.0000

Bcc 0.1781 6.869 2.451 2.291 -0.0743 0.9972 0.0000

Baa -0.0507 -6.799 -2.426 -2.268 0.7361 0.0396 0.6757

24 C(13) Bbb -0.0456 -6.119 -2.183 -2.041 -0.6746 -0.0390 0.7371

Bcc 0.0963 12.918 4.609 4.309 -0.0556 0.9985 0.0020

Baa -0.0039 -0.526 -0.188 -0.175 -0.5503 0.6443 -0.5311

25 C(13) Bbb 0.0002 0.030 0.011 0.010 0.4485 0.7646 0.4628

Bcc 0.0037 0.496 0.177 0.165 -0.7043 -0.0165 0.7098

Baa -0.0047 -0.637 -0.227 -0.213 0.0026 0.8895 0.4570

26 C(13) Bbb -0.0023 -0.302 -0.108 -0.101 -0.2828 -0.4377 0.8535

Bcc 0.0070 0.940 0.335 0.313 0.9592 -0.1314 0.2504

Baa -0.0020 -0.267 -0.095 -0.089 0.3563 -0.5163 0.7788

27 C(13) Bbb -0.0003 -0.044 -0.016 -0.015 0.2392 0.8561 0.4581

Bcc 0.0023 0.311 0.111 0.104 0.9032 -0.0230 -0.4285

Baa -0.0029 -0.384 -0.137 -0.128 0.3381 0.8585 0.3854

28 C(13) Bbb -0.0015 -0.202 -0.072 -0.067 0.7523 -0.0006 -0.6588

Bcc 0.0044 0.585 0.209 0.195 0.5654 -0.5127 0.6461

Baa -0.0011 -0.148 -0.053 -0.049 0.3112 -0.1208 0.9426

29 C(13) Bbb -0.0006 -0.086 -0.031 -0.029 0.4164 0.9089 -0.0210

Bcc 0.0017 0.234 0.083 0.078 0.8543 -0.3991 -0.3332

Baa -0.0042 -0.565 -0.202 -0.188 0.1810 0.8809 -0.4374

30 C(13) Bbb -0.0003 -0.042 -0.015 -0.014 0.9033 -0.3248 -0.2803

Bcc 0.0045 0.607 0.217 0.202 0.3890 0.3444 0.8545

Baa -0.0029 -0.384 -0.137 -0.128 0.3381 0.8585 -0.3854

31 C(13) Bbb -0.0015 -0.202 -0.072 -0.067 0.7523 -0.0006 0.6588

Bcc 0.0044 0.585 0.209 0.195 -0.5654 0.5127 0.6461

Baa -0.0020 -0.267 -0.095 -0.089 -0.3563 0.5163 0.7788

32 C(13) Bbb -0.0003 -0.044 -0.016 -0.015 0.2392 0.8561 -0.4581

Bcc 0.0023 0.311 0.111 0.104 0.9032 -0.0230 0.4285

Baa -0.0047 -0.637 -0.227 -0.213 0.0026 0.8895 -0.4570

33 C(13) Bbb -0.0023 -0.302 -0.108 -0.101 0.2828 0.4377 0.8535

Bcc 0.0070 0.940 0.335 0.313 0.9592 -0.1314 -0.2504

Baa -0.0039 -0.526 -0.188 -0.175 -0.5503 0.6443 0.5311

34 C(13) Bbb 0.0002 0.030 0.011 0.010 0.4485 0.7646 -0.4628

Bcc 0.0037 0.496 0.177 0.165 0.7043 0.0165 0.7098

Baa -0.0042 -0.565 -0.202 -0.188 0.1810 0.8809 0.4374

35 C(13) Bbb -0.0003 -0.042 -0.015 -0.014 0.9033 -0.3248 0.2803

Bcc 0.0045 0.607 0.217 0.202 -0.3890 -0.3444 0.8545

Baa -0.0011 -0.148 -0.053 -0.049 -0.3112 0.1208 0.9426

36 C(13) Bbb -0.0006 -0.086 -0.031 -0.029 0.4164 0.9089 0.0210

Bcc 0.0017 0.234 0.083 0.078 0.8543 -0.3991 0.3332

Baa -0.0039 -0.525 -0.187 -0.175 0.5504 0.6442 -0.5311

37 C(13) Bbb 0.0002 0.030 0.011 0.010 -0.4485 0.7647 0.4628

Bcc 0.0037 0.496 0.177 0.165 0.7042 -0.0165 0.7098

Baa -0.0042 -0.565 -0.202 -0.188 -0.1809 0.8808 -0.4375

38 C(13) Bbb -0.0003 -0.042 -0.015 -0.014 0.9034 0.3246 0.2800

Bcc 0.0045 0.607 0.217 0.202 -0.3886 0.3446 0.8545

Baa -0.0011 -0.148 -0.053 -0.049 -0.3111 -0.1207 0.9427

39 C(13) Bbb -0.0006 -0.086 -0.031 -0.029 -0.4164 0.9090 -0.0211

Bcc 0.0017 0.234 0.083 0.078 0.8543 0.3991 0.3330

Baa -0.0029 -0.384 -0.137 -0.128 -0.3381 0.8586 0.3854

40 C(13) Bbb -0.0015 -0.201 -0.072 -0.067 0.7523 0.0005 0.6588

Bcc 0.0044 0.585 0.209 0.195 -0.5654 -0.5126 0.6461

Baa -0.0020 -0.267 -0.095 -0.089 -0.3563 -0.5162 0.7789

41 C(13) Bbb -0.0003 -0.044 -0.016 -0.015 -0.2391 0.8562 0.4580

Bcc 0.0023 0.311 0.111 0.104 0.9033 0.0230 0.4284

Baa -0.0047 -0.637 -0.227 -0.213 -0.0025 0.8895 0.4569

42 C(13) Bbb -0.0023 -0.302 -0.108 -0.101 0.2826 -0.4377 0.8536

Bcc 0.0070 0.939 0.335 0.313 0.9592 0.1313 -0.2503

Baa -0.0039 -0.525 -0.187 -0.175 0.5504 0.6442 0.5311

43 C(13) Bbb 0.0002 0.030 0.011 0.010 -0.4485 0.7647 -0.4628

Bcc 0.0037 0.496 0.177 0.165 -0.7042 0.0165 0.7098

Baa -0.0042 -0.565 -0.202 -0.188 -0.1809 0.8808 0.4375

44 C(13) Bbb -0.0003 -0.042 -0.015 -0.014 0.9034 0.3246 -0.2800

Bcc 0.0045 0.607 0.217 0.202 0.3886 -0.3446 0.8545

Baa -0.0011 -0.148 -0.053 -0.049 0.3111 0.1207 0.9427

45 C(13) Bbb -0.0006 -0.086 -0.031 -0.029 -0.4164 0.9090 0.0211

Bcc 0.0017 0.234 0.083 0.078 0.8543 0.3991 -0.3330

Baa -0.0029 -0.384 -0.137 -0.128 -0.3381 0.8586 -0.3854

46 C(13) Bbb -0.0015 -0.201 -0.072 -0.067 0.7523 0.0005 -0.6588

Bcc 0.0044 0.585 0.209 0.195 0.5654 0.5126 0.6461

Baa -0.0020 -0.267 -0.095 -0.089 0.3563 0.5162 0.7789

47 C(13) Bbb -0.0003 -0.044 -0.016 -0.015 -0.2391 0.8562 -0.4580

Bcc 0.0023 0.311 0.111 0.104 0.9033 0.0230 -0.4284

Baa -0.0047 -0.637 -0.227 -0.213 -0.0025 0.8895 -0.4569

48 C(13) Bbb -0.0023 -0.302 -0.108 -0.101 -0.2826 0.4377 0.8536

Bcc 0.0070 0.939 0.335 0.313 0.9592 0.1313 0.2503

Baa -0.0014 -0.760 -0.271 -0.254 0.1101 0.9939 -0.0044

49 H(1) Bbb 0.0001 0.054 0.019 0.018 -0.2240 0.0291 0.9741

Bcc 0.0013 0.707 0.252 0.236 0.9683 -0.1063 0.2259

Baa -0.0014 -0.760 -0.271 -0.254 0.1101 0.9939 0.0044

50 H(1) Bbb 0.0001 0.054 0.019 0.018 0.2240 -0.0291 0.9741

Bcc 0.0013 0.707 0.252 0.236 0.9683 -0.1063 -0.2259

Baa -0.0060 -3.199 -1.142 -1.067 0.8748 0.1043 -0.4731

51 H(1) Bbb -0.0021 -1.119 -0.399 -0.373 -0.0250 0.9849 0.1711

Bcc 0.0081 4.319 1.541 1.441 0.4838 -0.1378 0.8642

Baa -0.0060 -3.199 -1.142 -1.067 0.8748 -0.1043 0.4731

52 H(1) Bbb -0.0021 -1.119 -0.399 -0.373 0.0249 0.9849 0.1711

Bcc 0.0081 4.319 1.541 1.441 -0.4839 -0.1379 0.8642

Baa -0.0060 -3.199 -1.142 -1.067 0.8748 -0.1043 -0.4731

53 H(1) Bbb -0.0021 -1.119 -0.399 -0.373 0.0249 0.9849 -0.1711

Bcc 0.0081 4.319 1.541 1.441 0.4839 0.1379 0.8642

Baa -0.0060 -3.199 -1.142 -1.067 0.8748 0.1043 0.4731

54 H(1) Bbb -0.0021 -1.119 -0.399 -0.373 -0.0250 0.9849 -0.1711

Bcc 0.0081 4.319 1.541 1.441 -0.4838 0.1378 0.8642

Baa -0.0014 -0.760 -0.271 -0.254 -0.1101 0.9939 -0.0044

55 H(1) Bbb 0.0001 0.054 0.019 0.018 0.2239 0.0291 0.9742

Bcc 0.0013 0.707 0.252 0.236 0.9684 0.1063 -0.2258

Baa -0.0014 -0.760 -0.271 -0.254 -0.1101 0.9939 0.0044

56 H(1) Bbb 0.0001 0.054 0.019 0.018 -0.2239 -0.0291 0.9742

Bcc 0.0013 0.707 0.252 0.236 0.9684 0.1063 0.2258

Baa -0.0015 -0.808 -0.288 -0.270 -0.6083 0.7821 -0.1357

57 H(1) Bbb -0.0004 -0.221 -0.079 -0.074 0.0841 0.2336 0.9687

Bcc 0.0019 1.030 0.367 0.343 0.7893 0.5778 -0.2078

Baa -0.0004 -0.219 -0.078 -0.073 0.5465 -0.4832 0.6839

58 H(1) Bbb -0.0003 -0.153 -0.055 -0.051 0.0236 0.8253 0.5642

Bcc 0.0007 0.373 0.133 0.124 0.8371 0.2922 -0.4625

Baa -0.0006 -0.310 -0.111 -0.104 0.3046 0.9243 0.2301

59 H(1) Bbb -0.0003 -0.147 -0.052 -0.049 0.5998 -0.3738 0.7074

Bcc 0.0009 0.457 0.163 0.152 0.7399 -0.0775 -0.6683

Baa -0.0005 -0.271 -0.097 -0.090 0.0994 0.8990 -0.4266

60 H(1) Bbb -0.0003 -0.177 -0.063 -0.059 0.7710 0.2014 0.6041

Bcc 0.0008 0.448 0.160 0.149 -0.6290 0.3890 0.6731

Baa -0.0013 -0.672 -0.240 -0.224 0.3271 0.7681 -0.5505

61 H(1) Bbb -0.0008 -0.445 -0.159 -0.148 0.7489 0.1446 0.6468

Bcc 0.0021 1.117 0.398 0.372 -0.5764 0.6237 0.5279

Baa -0.0006 -0.310 -0.111 -0.104 0.3046 0.9243 -0.2301

62 H(1) Bbb -0.0003 -0.147 -0.052 -0.049 -0.5998 0.3738 0.7074

Bcc 0.0009 0.457 0.163 0.152 0.7399 -0.0775 0.6683

Baa -0.0004 -0.219 -0.078 -0.073 -0.5465 0.4832 0.6839

63 H(1) Bbb -0.0003 -0.153 -0.055 -0.051 0.0236 0.8253 -0.5642

Bcc 0.0007 0.373 0.133 0.124 0.8371 0.2922 0.4625

Baa -0.0015 -0.808 -0.288 -0.270 -0.6083 0.7821 0.1357

64 H(1) Bbb -0.0004 -0.221 -0.079 -0.074 -0.0841 -0.2336 0.9687

Bcc 0.0019 1.030 0.367 0.343 0.7893 0.5778 0.2078

Baa -0.0013 -0.672 -0.240 -0.224 0.3271 0.7681 0.5505

65 H(1) Bbb -0.0008 -0.445 -0.159 -0.148 0.7489 0.1446 -0.6468

Bcc 0.0021 1.117 0.398 0.372 -0.5764 0.6237 -0.5279

Baa -0.0005 -0.271 -0.097 -0.090 0.0994 0.8990 0.4266

66 H(1) Bbb -0.0003 -0.177 -0.063 -0.059 0.7710 0.2014 -0.6041

Bcc 0.0008 0.448 0.160 0.149 0.6290 -0.3890 0.6731

Baa -0.0013 -0.672 -0.240 -0.224 -0.3271 0.7681 -0.5504

67 H(1) Bbb -0.0008 -0.445 -0.159 -0.148 0.7488 -0.1446 -0.6468

Bcc 0.0021 1.117 0.398 0.372 0.5764 0.6238 0.5279

Baa -0.0005 -0.271 -0.097 -0.090 -0.0995 0.8990 -0.4266

68 H(1) Bbb -0.0003 -0.177 -0.063 -0.059 0.7710 -0.2014 -0.6042

Bcc 0.0008 0.448 0.160 0.149 0.6290 0.3890 0.6730

Baa -0.0006 -0.310 -0.111 -0.103 -0.3045 0.9243 0.2300

69 H(1) Bbb -0.0003 -0.147 -0.052 -0.049 -0.5998 -0.3737 0.7075

Bcc 0.0009 0.457 0.163 0.152 0.7399 0.0775 0.6682

Baa -0.0004 -0.219 -0.078 -0.073 -0.5466 -0.4831 0.6840

70 H(1) Bbb -0.0003 -0.153 -0.055 -0.051 -0.0235 0.8254 0.5641

Bcc 0.0007 0.373 0.133 0.124 0.8371 -0.2922 0.4625

Baa -0.0015 -0.808 -0.288 -0.270 0.6083 0.7820 -0.1358

71 H(1) Bbb -0.0004 -0.221 -0.079 -0.074 -0.0841 0.2336 0.9687

Bcc 0.0019 1.030 0.367 0.343 0.7892 -0.5778 0.2079

Baa -0.0013 -0.672 -0.240 -0.224 -0.3271 0.7681 0.5504

72 H(1) Bbb -0.0008 -0.445 -0.159 -0.148 0.7488 -0.1446 0.6468

Bcc 0.0021 1.117 0.398 0.372 0.5764 0.6238 -0.5279

Baa -0.0005 -0.271 -0.097 -0.090 -0.0995 0.8990 0.4266

73 H(1) Bbb -0.0003 -0.177 -0.063 -0.059 0.7710 -0.2014 0.6042

Bcc 0.0008 0.448 0.160 0.149 -0.6290 -0.3890 0.6730

Baa -0.0006 -0.310 -0.111 -0.103 -0.3045 0.9243 -0.2300

74 H(1) Bbb -0.0003 -0.147 -0.052 -0.049 0.5998 0.3737 0.7075

Bcc 0.0009 0.457 0.163 0.152 0.7399 0.0775 -0.6682

Baa -0.0004 -0.219 -0.078 -0.073 0.5466 0.4831 0.6840

75 H(1) Bbb -0.0003 -0.153 -0.055 -0.051 -0.0235 0.8254 -0.5641

Bcc 0.0007 0.373 0.133 0.124 0.8371 -0.2922 -0.4625

Baa -0.0015 -0.808 -0.288 -0.270 0.6083 0.7820 0.1358

76 H(1) Bbb -0.0004 -0.221 -0.079 -0.074 0.0841 -0.2336 0.9687

Bcc 0.0019 1.030 0.367 0.343 0.7892 -0.5778 -0.2079

Baa -0.0050 -2.651 -0.946 -0.884 0.0000 -0.0000 1.0000

77 H(1) Bbb -0.0043 -2.297 -0.820 -0.766 0.0477 0.9989 0.0000

Bcc 0.0093 4.948 1.766 1.650 0.9989 -0.0477 -0.0000

Baa -0.0050 -2.652 -0.946 -0.884 0.0000 -0.0000 1.0000

78 H(1) Bbb -0.0043 -2.297 -0.819 -0.766 -0.0480 0.9988 0.0000

Bcc 0.0093 4.948 1.766 1.651 0.9988 0.0480 -0.0000

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

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Sun Aug 18 15:08:21 2019, MaxMem= 2013265920 cpu: 32.0

(Enter /home/kira/g09/l9999.exe)

1\1\ WCSS.PL-BEM-DHCP-129-94-99-158\FOpt\UB3LYP\6-311G(d)\C44H30N4(1-,

2)\KIRA\18-Aug-2019\0\\#p opt b3lyp/6-311G\* scrf=(solvent=dmso,smd) em

piricaldispersion=gd3bj\\TPPanion\\-1,2\C,4.2595619493,-0.1328455408,0

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.0628547672,0.000000039\C,2.8981078177,-0.0039251656,-1.1421736341\C,4

.2595619744,-0.1328455408,-0.6809410588\C,2.4606195383,0.0306256115,-2

.4563614817\C,1.0953365741,0.0922854613,-2.8786939189\N,0.0000556633,0

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AN AIRPLANE IS A COLLECTION OF SPARE PARTS

FLYING IN CLOSE FORMATION.

Job cpu time: 0 days 11 hours 34 minutes 6.9 seconds.

File lengths (MBytes): RWF= 1963 Int= 0 D2E= 0 Chk= 87 Scr= 1

Normal termination of Gaussian 09 at Sun Aug 18 15:08:22 2019.