Entering Gaussian System, Link 0=g09

Initial command:

/apps/gaussian/g09d01/g09/l1.exe "/srv/scratch/z5105842/Gau-150928.inp" -scrdir="/srv/scratch/z5105842/"

Entering Link 1 = /apps/gaussian/g09d01/g09/l1.exe PID= 150947.

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Cite this work as:

Gaussian 09, Revision D.01,

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

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

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

15-Jun-2019

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

%nprocshared=12

Will use up to 12 processors via shared memory.

%mem=10GB

%chk=ZnPCanion.chk

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

#p opt b3lyp/genecp 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=7,11=2,16=1,17=8,25=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=7,6=1,11=2,16=1,17=8,25=1,30=1,70=32205,71=1,72=21,74=-5,82=7,124=41/1,2,3;

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

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

7//1,2,3,16;

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

2/9=110/2;

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

99/9=1/99;

Leave Link 1 at Sat Jun 15 12:04:59 2019, MaxMem= 1342177280 cpu: 3.8

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

---------

ZnPCanion

---------

Symbolic Z-matrix:

Charge = -1 Multiplicity = 2

C 2.77772 1.18839 0.00238

N 1.43982 1.42409 0.02902

C 1.19044 2.7894 0.00284

C 2.47021 3.48217 -0.03695

C 3.4749 2.47654 -0.03787

N 0. 3.38988 -0.00476

C -1.19044 2.7894 0.00284

N -1.43982 1.42409 0.02902

C -2.77772 1.18839 0.00238

C -3.4749 2.47654 -0.03787

C -2.47021 3.48217 -0.03695

N 3.41035 0. -0.00133

C 3.4749 -2.47654 -0.03787

C 2.47021 -3.48217 -0.03695

C 1.19044 -2.7894 0.00284

N 1.43982 -1.42409 0.02902

C 2.77772 -1.18839 0.00238

N 0. -3.38988 -0.00476

N -1.43982 -1.42409 0.02902

C -1.19044 -2.7894 0.00284

C -2.47021 -3.48217 -0.03695

C -3.4749 -2.47654 -0.03787

C -2.77772 -1.18839 0.00238

N -3.41035 0. -0.00133

Zn 0. 0. 0.39114

C 4.8309 -2.81442 -0.07679

C 5.17488 -4.16759 -0.11147

C 4.17839 -5.16736 -0.11161

C 2.82276 -4.83751 -0.07683

C -4.8309 -2.81442 -0.07679

C -5.17488 -4.16759 -0.11147

C -4.17839 -5.16736 -0.11161

C -2.82276 -4.83751 -0.07683

C -2.82276 4.83751 -0.07683

C -4.17839 5.16736 -0.11161

C -5.17488 4.16759 -0.11147

C -4.8309 2.81442 -0.07679

C 4.8309 2.81442 -0.07679

C 5.17488 4.16759 -0.11147

C 4.17839 5.16736 -0.11161

C 2.82276 4.83751 -0.07683

H 5.59625 -2.04351 -0.07919

H 2.06073 -5.61165 -0.07925

H -5.59625 -2.04351 -0.07919

H -2.06073 -5.61165 -0.07925

H -2.06073 5.61165 -0.07925

H -5.59625 2.04351 -0.07919

H 5.59625 2.04351 -0.07919

H 2.06073 5.61165 -0.07925

H -4.4751 6.21221 -0.13972

H -6.22124 4.45784 -0.13949

H 4.4751 6.21221 -0.13972

H 6.22124 4.45784 -0.13949

H 6.22124 -4.45784 -0.13949

H 4.4751 -6.21221 -0.13972

H -4.4751 -6.21221 -0.13972

H -6.22124 -4.45784 -0.13949

NAtoms= 57 NQM= 57 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 14 12 12 12 14 12 14 12 12

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

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

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

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

Atom 11 12 13 14 15 16 17 18 19 20

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

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

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

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

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

Atom 21 22 23 24 25 26 27 28 29 30

IAtWgt= 12 12 12 14 64 12 12 12 12 12

AtmWgt= 12.0000000 12.0000000 12.0000000 14.0030740 63.9291454 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000

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

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

AtZNuc= 6.0000000 6.0000000 6.0000000 7.0000000 30.0000000 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 1 1 1 1 1 1 1 1 1

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

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

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

Atom 51 52 53 54 55 56 57

IAtWgt= 1 1 1 1 1 1 1

AtmWgt= 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250

NucSpn= 1 1 1 1 1 1 1

AtZEff= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NMagM= 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460

AtZNuc= 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000

Leave Link 101 at Sat Jun 15 12:04:59 2019, MaxMem= 1342177280 cpu: 5.4

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Initialization pass.

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

! Initial Parameters !

! (Angstroms and Degrees) !

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

! Name Definition Value Derivative Info. !

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

! R1 R(1,2) 1.3588 estimate D2E/DX2 !

! R2 R(1,5) 1.4653 estimate D2E/DX2 !

! R3 R(1,12) 1.3463 estimate D2E/DX2 !

! R4 R(2,3) 1.3881 estimate D2E/DX2 !

! R5 R(2,25) 2.0572 estimate D2E/DX2 !

! R6 R(3,4) 1.4558 estimate D2E/DX2 !

! R7 R(3,6) 1.3333 estimate D2E/DX2 !

! R8 R(4,5) 1.4215 estimate D2E/DX2 !

! R9 R(4,41) 1.401 estimate D2E/DX2 !

! R10 R(5,38) 1.398 estimate D2E/DX2 !

! R11 R(6,7) 1.3333 estimate D2E/DX2 !

! R12 R(7,8) 1.3881 estimate D2E/DX2 !

! R13 R(7,11) 1.4558 estimate D2E/DX2 !

! R14 R(8,9) 1.3588 estimate D2E/DX2 !

! R15 R(8,25) 2.0572 estimate D2E/DX2 !

! R16 R(9,10) 1.4653 estimate D2E/DX2 !

! R17 R(9,24) 1.3463 estimate D2E/DX2 !

! R18 R(10,11) 1.4215 estimate D2E/DX2 !

! R19 R(10,37) 1.398 estimate D2E/DX2 !

! R20 R(11,34) 1.401 estimate D2E/DX2 !

! R21 R(12,17) 1.3463 estimate D2E/DX2 !

! R22 R(13,14) 1.4215 estimate D2E/DX2 !

! R23 R(13,17) 1.4653 estimate D2E/DX2 !

! R24 R(13,26) 1.398 estimate D2E/DX2 !

! R25 R(14,15) 1.4558 estimate D2E/DX2 !

! R26 R(14,29) 1.401 estimate D2E/DX2 !

! R27 R(15,16) 1.3881 estimate D2E/DX2 !

! R28 R(15,18) 1.3333 estimate D2E/DX2 !

! R29 R(16,17) 1.3588 estimate D2E/DX2 !

! R30 R(16,25) 2.0572 estimate D2E/DX2 !

! R31 R(18,20) 1.3333 estimate D2E/DX2 !

! R32 R(19,20) 1.3881 estimate D2E/DX2 !

! R33 R(19,23) 1.3588 estimate D2E/DX2 !

! R34 R(19,25) 2.0572 estimate D2E/DX2 !

! R35 R(20,21) 1.4558 estimate D2E/DX2 !

! R36 R(21,22) 1.4215 estimate D2E/DX2 !

! R37 R(21,33) 1.401 estimate D2E/DX2 !

! R38 R(22,23) 1.4653 estimate D2E/DX2 !

! R39 R(22,30) 1.398 estimate D2E/DX2 !

! R40 R(23,24) 1.3463 estimate D2E/DX2 !

! R41 R(26,27) 1.3966 estimate D2E/DX2 !

! R42 R(26,42) 1.0863 estimate D2E/DX2 !

! R43 R(27,28) 1.4116 estimate D2E/DX2 !

! R44 R(27,54) 1.0862 estimate D2E/DX2 !

! R45 R(28,29) 1.3956 estimate D2E/DX2 !

! R46 R(28,55) 1.0865 estimate D2E/DX2 !

! R47 R(29,43) 1.0863 estimate D2E/DX2 !

! R48 R(30,31) 1.3966 estimate D2E/DX2 !

! R49 R(30,44) 1.0863 estimate D2E/DX2 !

! R50 R(31,32) 1.4116 estimate D2E/DX2 !

! R51 R(31,57) 1.0862 estimate D2E/DX2 !

! R52 R(32,33) 1.3956 estimate D2E/DX2 !

! R53 R(32,56) 1.0865 estimate D2E/DX2 !

! R54 R(33,45) 1.0863 estimate D2E/DX2 !

! R55 R(34,35) 1.3956 estimate D2E/DX2 !

! R56 R(34,46) 1.0863 estimate D2E/DX2 !

! R57 R(35,36) 1.4116 estimate D2E/DX2 !

! R58 R(35,50) 1.0865 estimate D2E/DX2 !

! R59 R(36,37) 1.3966 estimate D2E/DX2 !

! R60 R(36,51) 1.0862 estimate D2E/DX2 !

! R61 R(37,47) 1.0863 estimate D2E/DX2 !

! R62 R(38,39) 1.3966 estimate D2E/DX2 !

! R63 R(38,48) 1.0863 estimate D2E/DX2 !

! R64 R(39,40) 1.4116 estimate D2E/DX2 !

! R65 R(39,53) 1.0862 estimate D2E/DX2 !

! R66 R(40,41) 1.3956 estimate D2E/DX2 !

! R67 R(40,52) 1.0865 estimate D2E/DX2 !

! R68 R(41,49) 1.0863 estimate D2E/DX2 !

! A1 A(2,1,5) 108.4535 estimate D2E/DX2 !

! A2 A(2,1,12) 128.0152 estimate D2E/DX2 !

! A3 A(5,1,12) 123.5285 estimate D2E/DX2 !

! A4 A(1,2,3) 110.3122 estimate D2E/DX2 !

! A5 A(1,2,25) 124.9247 estimate D2E/DX2 !

! A6 A(3,2,25) 123.9476 estimate D2E/DX2 !

! A7 A(2,3,4) 108.0969 estimate D2E/DX2 !

! A8 A(2,3,6) 127.1178 estimate D2E/DX2 !

! A9 A(4,3,6) 124.779 estimate D2E/DX2 !

! A10 A(3,4,5) 106.5407 estimate D2E/DX2 !

! A11 A(3,4,41) 133.027 estimate D2E/DX2 !

! A12 A(5,4,41) 120.4315 estimate D2E/DX2 !

! A13 A(1,5,4) 106.5958 estimate D2E/DX2 !

! A14 A(1,5,38) 132.4343 estimate D2E/DX2 !

! A15 A(4,5,38) 120.9696 estimate D2E/DX2 !

! A16 A(3,6,7) 126.4617 estimate D2E/DX2 !

! A17 A(6,7,8) 127.1178 estimate D2E/DX2 !

! A18 A(6,7,11) 124.779 estimate D2E/DX2 !

! A19 A(8,7,11) 108.0969 estimate D2E/DX2 !

! A20 A(7,8,9) 110.3122 estimate D2E/DX2 !

! A21 A(7,8,25) 123.9476 estimate D2E/DX2 !

! A22 A(9,8,25) 124.9247 estimate D2E/DX2 !

! A23 A(8,9,10) 108.4535 estimate D2E/DX2 !

! A24 A(8,9,24) 128.0152 estimate D2E/DX2 !

! A25 A(10,9,24) 123.5285 estimate D2E/DX2 !

! A26 A(9,10,11) 106.5958 estimate D2E/DX2 !

! A27 A(9,10,37) 132.4343 estimate D2E/DX2 !

! A28 A(11,10,37) 120.9696 estimate D2E/DX2 !

! A29 A(7,11,10) 106.5407 estimate D2E/DX2 !

! A30 A(7,11,34) 133.027 estimate D2E/DX2 !

! A31 A(10,11,34) 120.4315 estimate D2E/DX2 !

! A32 A(1,12,17) 123.9421 estimate D2E/DX2 !

! A33 A(14,13,17) 106.5958 estimate D2E/DX2 !

! A34 A(14,13,26) 120.9696 estimate D2E/DX2 !

! A35 A(17,13,26) 132.4343 estimate D2E/DX2 !

! A36 A(13,14,15) 106.5407 estimate D2E/DX2 !

! A37 A(13,14,29) 120.4315 estimate D2E/DX2 !

! A38 A(15,14,29) 133.027 estimate D2E/DX2 !

! A39 A(14,15,16) 108.0969 estimate D2E/DX2 !

! A40 A(14,15,18) 124.779 estimate D2E/DX2 !

! A41 A(16,15,18) 127.1178 estimate D2E/DX2 !

! A42 A(15,16,17) 110.3122 estimate D2E/DX2 !

! A43 A(15,16,25) 123.9476 estimate D2E/DX2 !

! A44 A(17,16,25) 124.9247 estimate D2E/DX2 !

! A45 A(12,17,13) 123.5285 estimate D2E/DX2 !

! A46 A(12,17,16) 128.0152 estimate D2E/DX2 !

! A47 A(13,17,16) 108.4535 estimate D2E/DX2 !

! A48 A(15,18,20) 126.4617 estimate D2E/DX2 !

! A49 A(20,19,23) 110.3122 estimate D2E/DX2 !

! A50 A(20,19,25) 123.9476 estimate D2E/DX2 !

! A51 A(23,19,25) 124.9247 estimate D2E/DX2 !

! A52 A(18,20,19) 127.1178 estimate D2E/DX2 !

! A53 A(18,20,21) 124.779 estimate D2E/DX2 !

! A54 A(19,20,21) 108.0969 estimate D2E/DX2 !

! A55 A(20,21,22) 106.5407 estimate D2E/DX2 !

! A56 A(20,21,33) 133.027 estimate D2E/DX2 !

! A57 A(22,21,33) 120.4315 estimate D2E/DX2 !

! A58 A(21,22,23) 106.5958 estimate D2E/DX2 !

! A59 A(21,22,30) 120.9696 estimate D2E/DX2 !

! A60 A(23,22,30) 132.4343 estimate D2E/DX2 !

! A61 A(19,23,22) 108.4535 estimate D2E/DX2 !

! A62 A(19,23,24) 128.0152 estimate D2E/DX2 !

! A63 A(22,23,24) 123.5285 estimate D2E/DX2 !

! A64 A(9,24,23) 123.9421 estimate D2E/DX2 !

! A65 A(2,25,8) 88.8342 estimate D2E/DX2 !

! A66 A(2,25,16) 87.6145 estimate D2E/DX2 !

! A67 A(2,25,19) 159.7235 estimate D2E/DX2 !

! A68 A(8,25,16) 159.7235 estimate D2E/DX2 !

! A69 A(8,25,19) 87.6145 estimate D2E/DX2 !

! A70 A(16,25,19) 88.8342 estimate D2E/DX2 !

! A71 A(13,26,27) 118.2777 estimate D2E/DX2 !

! A72 A(13,26,42) 120.7915 estimate D2E/DX2 !

! A73 A(27,26,42) 120.9307 estimate D2E/DX2 !

! A74 A(26,27,28) 120.8215 estimate D2E/DX2 !

! A75 A(26,27,54) 119.7877 estimate D2E/DX2 !

! A76 A(28,27,54) 119.3908 estimate D2E/DX2 !

! A77 A(27,28,29) 121.2194 estimate D2E/DX2 !

! A78 A(27,28,55) 119.2308 estimate D2E/DX2 !

! A79 A(29,28,55) 119.5498 estimate D2E/DX2 !

! A80 A(14,29,28) 118.2796 estimate D2E/DX2 !

! A81 A(14,29,43) 120.8617 estimate D2E/DX2 !

! A82 A(28,29,43) 120.8587 estimate D2E/DX2 !

! A83 A(22,30,31) 118.2777 estimate D2E/DX2 !

! A84 A(22,30,44) 120.7915 estimate D2E/DX2 !

! A85 A(31,30,44) 120.9307 estimate D2E/DX2 !

! A86 A(30,31,32) 120.8215 estimate D2E/DX2 !

! A87 A(30,31,57) 119.7877 estimate D2E/DX2 !

! A88 A(32,31,57) 119.3908 estimate D2E/DX2 !

! A89 A(31,32,33) 121.2194 estimate D2E/DX2 !

! A90 A(31,32,56) 119.2308 estimate D2E/DX2 !

! A91 A(33,32,56) 119.5498 estimate D2E/DX2 !

! A92 A(21,33,32) 118.2796 estimate D2E/DX2 !

! A93 A(21,33,45) 120.8617 estimate D2E/DX2 !

! A94 A(32,33,45) 120.8587 estimate D2E/DX2 !

! A95 A(11,34,35) 118.2796 estimate D2E/DX2 !

! A96 A(11,34,46) 120.8617 estimate D2E/DX2 !

! A97 A(35,34,46) 120.8587 estimate D2E/DX2 !

! A98 A(34,35,36) 121.2194 estimate D2E/DX2 !

! A99 A(34,35,50) 119.5498 estimate D2E/DX2 !

! A100 A(36,35,50) 119.2308 estimate D2E/DX2 !

! A101 A(35,36,37) 120.8215 estimate D2E/DX2 !

! A102 A(35,36,51) 119.3908 estimate D2E/DX2 !

! A103 A(37,36,51) 119.7877 estimate D2E/DX2 !

! A104 A(10,37,36) 118.2777 estimate D2E/DX2 !

! A105 A(10,37,47) 120.7915 estimate D2E/DX2 !

! A106 A(36,37,47) 120.9307 estimate D2E/DX2 !

! A107 A(5,38,39) 118.2777 estimate D2E/DX2 !

! A108 A(5,38,48) 120.7915 estimate D2E/DX2 !

! A109 A(39,38,48) 120.9307 estimate D2E/DX2 !

! A110 A(38,39,40) 120.8215 estimate D2E/DX2 !

! A111 A(38,39,53) 119.7877 estimate D2E/DX2 !

! A112 A(40,39,53) 119.3908 estimate D2E/DX2 !

! A113 A(39,40,41) 121.2194 estimate D2E/DX2 !

! A114 A(39,40,52) 119.2308 estimate D2E/DX2 !

! A115 A(41,40,52) 119.5498 estimate D2E/DX2 !

! A116 A(4,41,40) 118.2796 estimate D2E/DX2 !

! A117 A(4,41,49) 120.8617 estimate D2E/DX2 !

! A118 A(40,41,49) 120.8587 estimate D2E/DX2 !

! D1 D(5,1,2,3) 0.2841 estimate D2E/DX2 !

! D2 D(5,1,2,25) -169.687 estimate D2E/DX2 !

! D3 D(12,1,2,3) -179.1098 estimate D2E/DX2 !

! D4 D(12,1,2,25) 10.9191 estimate D2E/DX2 !

! D5 D(2,1,5,4) -0.1514 estimate D2E/DX2 !

! D6 D(2,1,5,38) -179.9368 estimate D2E/DX2 !

! D7 D(12,1,5,4) 179.2758 estimate D2E/DX2 !

! D8 D(12,1,5,38) -0.5097 estimate D2E/DX2 !

! D9 D(2,1,12,17) 1.007 estimate D2E/DX2 !

! D10 D(5,1,12,17) -178.3033 estimate D2E/DX2 !

! D11 D(1,2,3,4) -0.3039 estimate D2E/DX2 !

! D12 D(1,2,3,6) 178.8099 estimate D2E/DX2 !

! D13 D(25,2,3,4) 169.7849 estimate D2E/DX2 !

! D14 D(25,2,3,6) -11.1013 estimate D2E/DX2 !

! D15 D(1,2,25,8) -175.6805 estimate D2E/DX2 !

! D16 D(1,2,25,16) -15.648 estimate D2E/DX2 !

! D17 D(1,2,25,19) -95.7716 estimate D2E/DX2 !

! D18 D(3,2,25,8) 15.6736 estimate D2E/DX2 !

! D19 D(3,2,25,16) 175.7062 estimate D2E/DX2 !

! D20 D(3,2,25,19) 95.5825 estimate D2E/DX2 !

! D21 D(2,3,4,5) 0.1991 estimate D2E/DX2 !

! D22 D(2,3,4,41) 179.8554 estimate D2E/DX2 !

! D23 D(6,3,4,5) -178.9406 estimate D2E/DX2 !

! D24 D(6,3,4,41) 0.7157 estimate D2E/DX2 !

! D25 D(2,3,6,7) -0.4607 estimate D2E/DX2 !

! D26 D(4,3,6,7) 178.5137 estimate D2E/DX2 !

! D27 D(3,4,5,1) -0.0309 estimate D2E/DX2 !

! D28 D(3,4,5,38) 179.7844 estimate D2E/DX2 !

! D29 D(41,4,5,1) -179.7395 estimate D2E/DX2 !

! D30 D(41,4,5,38) 0.0758 estimate D2E/DX2 !

! D31 D(3,4,41,40) -179.8756 estimate D2E/DX2 !

! D32 D(3,4,41,49) 0.2065 estimate D2E/DX2 !

! D33 D(5,4,41,40) -0.2578 estimate D2E/DX2 !

! D34 D(5,4,41,49) 179.8244 estimate D2E/DX2 !

! D35 D(1,5,38,39) 179.9166 estimate D2E/DX2 !

! D36 D(1,5,38,48) -0.1291 estimate D2E/DX2 !

! D37 D(4,5,38,39) 0.1564 estimate D2E/DX2 !

! D38 D(4,5,38,48) -179.8893 estimate D2E/DX2 !

! D39 D(3,6,7,8) 0.4607 estimate D2E/DX2 !

! D40 D(3,6,7,11) -178.5137 estimate D2E/DX2 !

! D41 D(6,7,8,9) -178.8099 estimate D2E/DX2 !

! D42 D(6,7,8,25) 11.1013 estimate D2E/DX2 !

! D43 D(11,7,8,9) 0.3039 estimate D2E/DX2 !

! D44 D(11,7,8,25) -169.7849 estimate D2E/DX2 !

! D45 D(6,7,11,10) 178.9406 estimate D2E/DX2 !

! D46 D(6,7,11,34) -0.7157 estimate D2E/DX2 !

! D47 D(8,7,11,10) -0.1991 estimate D2E/DX2 !

! D48 D(8,7,11,34) -179.8554 estimate D2E/DX2 !

! D49 D(7,8,9,10) -0.2841 estimate D2E/DX2 !

! D50 D(7,8,9,24) 179.1098 estimate D2E/DX2 !

! D51 D(25,8,9,10) 169.687 estimate D2E/DX2 !

! D52 D(25,8,9,24) -10.9191 estimate D2E/DX2 !

! D53 D(7,8,25,2) -15.6736 estimate D2E/DX2 !

! D54 D(7,8,25,16) -95.5825 estimate D2E/DX2 !

! D55 D(7,8,25,19) -175.7062 estimate D2E/DX2 !

! D56 D(9,8,25,2) 175.6805 estimate D2E/DX2 !

! D57 D(9,8,25,16) 95.7716 estimate D2E/DX2 !

! D58 D(9,8,25,19) 15.648 estimate D2E/DX2 !

! D59 D(8,9,10,11) 0.1514 estimate D2E/DX2 !

! D60 D(8,9,10,37) 179.9368 estimate D2E/DX2 !

! D61 D(24,9,10,11) -179.2758 estimate D2E/DX2 !

! D62 D(24,9,10,37) 0.5097 estimate D2E/DX2 !

! D63 D(8,9,24,23) -1.007 estimate D2E/DX2 !

! D64 D(10,9,24,23) 178.3033 estimate D2E/DX2 !

! D65 D(9,10,11,7) 0.0309 estimate D2E/DX2 !

! D66 D(9,10,11,34) 179.7395 estimate D2E/DX2 !

! D67 D(37,10,11,7) -179.7844 estimate D2E/DX2 !

! D68 D(37,10,11,34) -0.0758 estimate D2E/DX2 !

! D69 D(9,10,37,36) -179.9166 estimate D2E/DX2 !

! D70 D(9,10,37,47) 0.1291 estimate D2E/DX2 !

! D71 D(11,10,37,36) -0.1564 estimate D2E/DX2 !

! D72 D(11,10,37,47) 179.8893 estimate D2E/DX2 !

! D73 D(7,11,34,35) 179.8756 estimate D2E/DX2 !

! D74 D(7,11,34,46) -0.2065 estimate D2E/DX2 !

! D75 D(10,11,34,35) 0.2578 estimate D2E/DX2 !

! D76 D(10,11,34,46) -179.8244 estimate D2E/DX2 !

! D77 D(1,12,17,13) 178.3033 estimate D2E/DX2 !

! D78 D(1,12,17,16) -1.007 estimate D2E/DX2 !

! D79 D(17,13,14,15) 0.0309 estimate D2E/DX2 !

! D80 D(17,13,14,29) 179.7395 estimate D2E/DX2 !

! D81 D(26,13,14,15) -179.7844 estimate D2E/DX2 !

! D82 D(26,13,14,29) -0.0758 estimate D2E/DX2 !

! D83 D(14,13,17,12) -179.2758 estimate D2E/DX2 !

! D84 D(14,13,17,16) 0.1514 estimate D2E/DX2 !

! D85 D(26,13,17,12) 0.5097 estimate D2E/DX2 !

! D86 D(26,13,17,16) 179.9368 estimate D2E/DX2 !

! D87 D(14,13,26,27) -0.1564 estimate D2E/DX2 !

! D88 D(14,13,26,42) 179.8893 estimate D2E/DX2 !

! D89 D(17,13,26,27) -179.9166 estimate D2E/DX2 !

! D90 D(17,13,26,42) 0.1291 estimate D2E/DX2 !

! D91 D(13,14,15,16) -0.1991 estimate D2E/DX2 !

! D92 D(13,14,15,18) 178.9406 estimate D2E/DX2 !

! D93 D(29,14,15,16) -179.8554 estimate D2E/DX2 !

! D94 D(29,14,15,18) -0.7157 estimate D2E/DX2 !

! D95 D(13,14,29,28) 0.2578 estimate D2E/DX2 !

! D96 D(13,14,29,43) -179.8244 estimate D2E/DX2 !

! D97 D(15,14,29,28) 179.8756 estimate D2E/DX2 !

! D98 D(15,14,29,43) -0.2065 estimate D2E/DX2 !

! D99 D(14,15,16,17) 0.3039 estimate D2E/DX2 !

! D100 D(14,15,16,25) -169.7849 estimate D2E/DX2 !

! D101 D(18,15,16,17) -178.8099 estimate D2E/DX2 !

! D102 D(18,15,16,25) 11.1013 estimate D2E/DX2 !

! D103 D(14,15,18,20) -178.5137 estimate D2E/DX2 !

! D104 D(16,15,18,20) 0.4607 estimate D2E/DX2 !

! D105 D(15,16,17,12) 179.1098 estimate D2E/DX2 !

! D106 D(15,16,17,13) -0.2841 estimate D2E/DX2 !

! D107 D(25,16,17,12) -10.9191 estimate D2E/DX2 !

! D108 D(25,16,17,13) 169.687 estimate D2E/DX2 !

! D109 D(15,16,25,2) -175.7062 estimate D2E/DX2 !

! D110 D(15,16,25,8) -95.5825 estimate D2E/DX2 !

! D111 D(15,16,25,19) -15.6736 estimate D2E/DX2 !

! D112 D(17,16,25,2) 15.648 estimate D2E/DX2 !

! D113 D(17,16,25,8) 95.7716 estimate D2E/DX2 !

! D114 D(17,16,25,19) 175.6805 estimate D2E/DX2 !

! D115 D(15,18,20,19) -0.4607 estimate D2E/DX2 !

! D116 D(15,18,20,21) 178.5137 estimate D2E/DX2 !

! D117 D(23,19,20,18) 178.8099 estimate D2E/DX2 !

! D118 D(23,19,20,21) -0.3039 estimate D2E/DX2 !

! D119 D(25,19,20,18) -11.1013 estimate D2E/DX2 !

! D120 D(25,19,20,21) 169.7849 estimate D2E/DX2 !

! D121 D(20,19,23,22) 0.2841 estimate D2E/DX2 !

! D122 D(20,19,23,24) -179.1098 estimate D2E/DX2 !

! D123 D(25,19,23,22) -169.687 estimate D2E/DX2 !

! D124 D(25,19,23,24) 10.9191 estimate D2E/DX2 !

! D125 D(20,19,25,2) 95.5825 estimate D2E/DX2 !

! D126 D(20,19,25,8) 175.7062 estimate D2E/DX2 !

! D127 D(20,19,25,16) 15.6736 estimate D2E/DX2 !

! D128 D(23,19,25,2) -95.7716 estimate D2E/DX2 !

! D129 D(23,19,25,8) -15.648 estimate D2E/DX2 !

! D130 D(23,19,25,16) -175.6805 estimate D2E/DX2 !

! D131 D(18,20,21,22) -178.9406 estimate D2E/DX2 !

! D132 D(18,20,21,33) 0.7157 estimate D2E/DX2 !

! D133 D(19,20,21,22) 0.1991 estimate D2E/DX2 !

! D134 D(19,20,21,33) 179.8554 estimate D2E/DX2 !

! D135 D(20,21,22,23) -0.0309 estimate D2E/DX2 !

! D136 D(20,21,22,30) 179.7844 estimate D2E/DX2 !

! D137 D(33,21,22,23) -179.7395 estimate D2E/DX2 !

! D138 D(33,21,22,30) 0.0758 estimate D2E/DX2 !

! D139 D(20,21,33,32) -179.8756 estimate D2E/DX2 !

! D140 D(20,21,33,45) 0.2065 estimate D2E/DX2 !

! D141 D(22,21,33,32) -0.2578 estimate D2E/DX2 !

! D142 D(22,21,33,45) 179.8244 estimate D2E/DX2 !

! D143 D(21,22,23,19) -0.1514 estimate D2E/DX2 !

! D144 D(21,22,23,24) 179.2758 estimate D2E/DX2 !

! D145 D(30,22,23,19) -179.9368 estimate D2E/DX2 !

! D146 D(30,22,23,24) -0.5097 estimate D2E/DX2 !

! D147 D(21,22,30,31) 0.1564 estimate D2E/DX2 !

! D148 D(21,22,30,44) -179.8893 estimate D2E/DX2 !

! D149 D(23,22,30,31) 179.9166 estimate D2E/DX2 !

! D150 D(23,22,30,44) -0.1291 estimate D2E/DX2 !

! D151 D(19,23,24,9) 1.007 estimate D2E/DX2 !

! D152 D(22,23,24,9) -178.3033 estimate D2E/DX2 !

! D153 D(13,26,27,28) 0.2038 estimate D2E/DX2 !

! D154 D(13,26,27,54) -179.8427 estimate D2E/DX2 !

! D155 D(42,26,27,28) -179.842 estimate D2E/DX2 !

! D156 D(42,26,27,54) 0.1116 estimate D2E/DX2 !

! D157 D(26,27,28,29) -0.0198 estimate D2E/DX2 !

! D158 D(26,27,28,55) 179.9579 estimate D2E/DX2 !

! D159 D(54,27,28,29) -179.9735 estimate D2E/DX2 !

! D160 D(54,27,28,55) 0.0042 estimate D2E/DX2 !

! D161 D(27,28,29,14) -0.2121 estimate D2E/DX2 !

! D162 D(27,28,29,43) 179.87 estimate D2E/DX2 !

! D163 D(55,28,29,14) 179.8102 estimate D2E/DX2 !

! D164 D(55,28,29,43) -0.1076 estimate D2E/DX2 !

! D165 D(22,30,31,32) -0.2038 estimate D2E/DX2 !

! D166 D(22,30,31,57) 179.8427 estimate D2E/DX2 !

! D167 D(44,30,31,32) 179.842 estimate D2E/DX2 !

! D168 D(44,30,31,57) -0.1116 estimate D2E/DX2 !

! D169 D(30,31,32,33) 0.0198 estimate D2E/DX2 !

! D170 D(30,31,32,56) -179.9579 estimate D2E/DX2 !

! D171 D(57,31,32,33) 179.9735 estimate D2E/DX2 !

! D172 D(57,31,32,56) -0.0042 estimate D2E/DX2 !

! D173 D(31,32,33,21) 0.2121 estimate D2E/DX2 !

! D174 D(31,32,33,45) -179.87 estimate D2E/DX2 !

! D175 D(56,32,33,21) -179.8102 estimate D2E/DX2 !

! D176 D(56,32,33,45) 0.1076 estimate D2E/DX2 !

! D177 D(11,34,35,36) -0.2121 estimate D2E/DX2 !

! D178 D(11,34,35,50) 179.8102 estimate D2E/DX2 !

! D179 D(46,34,35,36) 179.87 estimate D2E/DX2 !

! D180 D(46,34,35,50) -0.1076 estimate D2E/DX2 !

! D181 D(34,35,36,37) -0.0198 estimate D2E/DX2 !

! D182 D(34,35,36,51) -179.9735 estimate D2E/DX2 !

! D183 D(50,35,36,37) 179.9579 estimate D2E/DX2 !

! D184 D(50,35,36,51) 0.0042 estimate D2E/DX2 !

! D185 D(35,36,37,10) 0.2038 estimate D2E/DX2 !

! D186 D(35,36,37,47) -179.842 estimate D2E/DX2 !

! D187 D(51,36,37,10) -179.8427 estimate D2E/DX2 !

! D188 D(51,36,37,47) 0.1116 estimate D2E/DX2 !

! D189 D(5,38,39,40) -0.2038 estimate D2E/DX2 !

! D190 D(5,38,39,53) 179.8427 estimate D2E/DX2 !

! D191 D(48,38,39,40) 179.842 estimate D2E/DX2 !

! D192 D(48,38,39,53) -0.1116 estimate D2E/DX2 !

! D193 D(38,39,40,41) 0.0198 estimate D2E/DX2 !

! D194 D(38,39,40,52) -179.9579 estimate D2E/DX2 !

! D195 D(53,39,40,41) 179.9735 estimate D2E/DX2 !

! D196 D(53,39,40,52) -0.0042 estimate D2E/DX2 !

! D197 D(39,40,41,4) 0.2121 estimate D2E/DX2 !

! D198 D(39,40,41,49) -179.87 estimate D2E/DX2 !

! D199 D(52,40,41,4) -179.8102 estimate D2E/DX2 !

! D200 D(52,40,41,49) 0.1076 estimate D2E/DX2 !

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

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

Number of steps in this run= 342 maximum allowed number of steps= 342.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jun 15 12:05:00 2019, MaxMem= 1342177280 cpu: 0.4

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

Stoichiometry C32H16N8Zn(1-,2)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C32H16N4)]

Deg. of freedom 43

Full point group C2V NOp 4

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 2.777717 1.188389 0.002377

2 7 0 1.439815 1.424093 0.029020

3 6 0 1.190436 2.789403 0.002839

4 6 0 2.470212 3.482165 -0.036946

5 6 0 3.474898 2.476544 -0.037870

6 7 0 0.000000 3.389883 -0.004761

7 6 0 -1.190436 2.789403 0.002839

8 7 0 -1.439815 1.424093 0.029020

9 6 0 -2.777717 1.188389 0.002377

10 6 0 -3.474898 2.476544 -0.037870

11 6 0 -2.470212 3.482165 -0.036946

12 7 0 3.410354 0.000000 -0.001325

13 6 0 3.474898 -2.476544 -0.037870

14 6 0 2.470212 -3.482165 -0.036946

15 6 0 1.190436 -2.789403 0.002839

16 7 0 1.439815 -1.424093 0.029020

17 6 0 2.777717 -1.188389 0.002377

18 7 0 0.000000 -3.389883 -0.004761

19 7 0 -1.439815 -1.424093 0.029020

20 6 0 -1.190436 -2.789403 0.002839

21 6 0 -2.470212 -3.482165 -0.036946

22 6 0 -3.474898 -2.476544 -0.037870

23 6 0 -2.777717 -1.188389 0.002377

24 7 0 -3.410354 0.000000 -0.001325

25 30 0 0.000000 0.000000 0.391144

26 6 0 4.830902 -2.814424 -0.076788

27 6 0 5.174876 -4.167586 -0.111467

28 6 0 4.178392 -5.167360 -0.111609

29 6 0 2.822756 -4.837513 -0.076831

30 6 0 -4.830902 -2.814424 -0.076788

31 6 0 -5.174876 -4.167586 -0.111467

32 6 0 -4.178392 -5.167360 -0.111609

33 6 0 -2.822756 -4.837513 -0.076831

34 6 0 -2.822756 4.837513 -0.076831

35 6 0 -4.178392 5.167360 -0.111609

36 6 0 -5.174876 4.167586 -0.111467

37 6 0 -4.830902 2.814424 -0.076788

38 6 0 4.830902 2.814424 -0.076788

39 6 0 5.174876 4.167586 -0.111467

40 6 0 4.178392 5.167360 -0.111609

41 6 0 2.822756 4.837513 -0.076831

42 1 0 5.596246 -2.043514 -0.079188

43 1 0 2.060727 -5.611653 -0.079254

44 1 0 -5.596246 -2.043514 -0.079188

45 1 0 -2.060727 -5.611653 -0.079254

46 1 0 -2.060727 5.611653 -0.079254

47 1 0 -5.596246 2.043514 -0.079188

48 1 0 5.596246 2.043514 -0.079188

49 1 0 2.060727 5.611653 -0.079254

50 1 0 -4.475100 6.212206 -0.139717

51 1 0 -6.221236 4.457844 -0.139486

52 1 0 4.475100 6.212206 -0.139717

53 1 0 6.221236 4.457844 -0.139486

54 1 0 6.221236 -4.457844 -0.139486

55 1 0 4.475100 -6.212206 -0.139717

56 1 0 -4.475100 -6.212206 -0.139717

57 1 0 -6.221236 -4.457844 -0.139486

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

Rotational constants (GHZ): 0.0876884 0.0875743 0.0439064

Leave Link 202 at Sat Jun 15 12:05:00 2019, MaxMem= 1342177280 cpu: 0.6

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

General basis read from cards: (5D, 7F)

Centers: 25

S 1 1.00

Exponent= 7.9970000000D-01 Coefficients= 1.0000000000D+00

S 1 1.00

Exponent= 1.7520000000D-01 Coefficients= 1.0000000000D+00

S 1 1.00

Exponent= 5.5600000000D-02 Coefficients= 1.0000000000D+00

P 1 1.00

Exponent= 1.2020000000D-01 Coefficients= 1.0000000000D+00

P 1 1.00

Exponent= 3.5100000000D-02 Coefficients= 1.0000000000D+00

D 3 1.00

Exponent= 6.8850000000D+01 Coefficients= 2.5853200000D-02

Exponent= 1.8320000000D+01 Coefficients= 1.6511950000D-01

Exponent= 5.9220000000D+00 Coefficients= 4.4682120000D-01

D 1 1.00

Exponent= 1.9270000000D+00 Coefficients= 1.0000000000D+00

D 1 1.00

Exponent= 5.5280000000D-01 Coefficients= 1.0000000000D+00

\*\*\*\*

Centers: 42 43 44 45 46 47 48 49 50 51

Centers: 52 53 54 55 56 57 1 3 4 5

Centers: 7 9 10 11 13 14 15 17 20 21

Centers: 22 23 26 27 28 29 30 31 32 33

Centers: 34 35 36 37 38 39 40 41 2 6

Centers: 8 12 16 18 19 24

6-311G\*

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

Pseudopotential Parameters

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

Center Atomic Valence Angular Power

Number Number Electrons Momentum of R Exponent Coefficient SO-Coeffient

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

1 6

No pseudopotential on this center.

2 7

No pseudopotential on this center.

3 6

No pseudopotential on this center.

4 6

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5 6

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19 7

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22 6

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23 6

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24 7

No pseudopotential on this center.

25 30 12

F and up

1 386.7379660 -18.00000000 0.00000000

2 72.8587359 -124.35274030 0.00000000

2 15.9066170 -30.66018220 0.00000000

2 4.3502340 -10.63589890 0.00000000

2 1.2842199 -0.76836230 0.00000000

S - F

0 19.0867858 3.00000000 0.00000000

1 5.0231080 22.52342250 0.00000000

2 1.2701744 48.44659420 0.00000000

2 1.0671287 -44.55601190 0.00000000

2 0.9264190 12.99839580 0.00000000

P - F

0 43.4927750 5.00000000 0.00000000

1 20.8692669 20.74355890 0.00000000

2 21.7118378 90.30271580 0.00000000

2 6.3616915 74.66103160 0.00000000

2 1.2291195 9.88944240 0.00000000

D - F

2 13.5851800 -4.84903590 0.00000000

2 9.8373050 3.69133790 0.00000000

2 0.8373113 -0.50373190 0.00000000

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57 1

No pseudopotential on this center.

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

There are 225 symmetry adapted cartesian basis functions of A1 symmetry.

There are 196 symmetry adapted cartesian basis functions of A2 symmetry.

There are 207 symmetry adapted cartesian basis functions of B1 symmetry.

There are 207 symmetry adapted cartesian basis functions of B2 symmetry.

There are 211 symmetry adapted basis functions of A1 symmetry.

There are 187 symmetry adapted basis functions of A2 symmetry.

There are 197 symmetry adapted basis functions of B1 symmetry.

There are 197 symmetry adapted basis functions of B2 symmetry.

792 basis functions, 1399 primitive gaussians, 835 cartesian basis functions

139 alpha electrons 138 beta electrons

nuclear repulsion energy 4365.2036725104 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= 57 NActive= 57 NUniq= 16 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1640381979 Hartrees.

Nuclear repulsion after empirical dispersion term = 4365.0396343124 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= 57.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 57

GePol: Total number of spheres = 57

GePol: Number of exposed spheres = 57 (100.00%)

GePol: Number of points = 4670

GePol: Average weight of points = 0.10

GePol: Minimum weight of points = 0.93D-09

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 312

GePol: Fraction of low-weight points (<1% of avg) = 6.68%

GePol: Cavity surface area = 486.913 Ang\*\*2

GePol: Cavity volume = 505.662 Ang\*\*3

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

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PCM non-electrostatic energy = -0.0143188439 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 4365.0253154685 Hartrees.

Leave Link 301 at Sat Jun 15 12:05:00 2019, MaxMem= 1342177280 cpu: 1.1

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 32896 NPrTT= 163506 LenC2= 22819 LenP2D= 61244.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 792 RedAO= T EigKep= 3.54D-05 NBF= 211 187 197 197

NBsUse= 792 1.00D-06 EigRej= -1.00D+00 NBFU= 211 187 197 197

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= 802 802 802 802 802 MxSgAt= 57 MxSgA2= 57.

Leave Link 302 at Sat Jun 15 12:05:01 2019, MaxMem= 1342177280 cpu: 12.6

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

DipDrv: MaxL=1.

Leave Link 303 at Sat Jun 15 12:05:02 2019, MaxMem= 1342177280 cpu: 4.0

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

ExpMin= 3.51D-02 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -1733.82812209577

JPrj=0 DoOrth=F DoCkMO=F.

Initial guess orbital symmetries:

Alpha Orbitals:

Occupied (B2) (B1) (A2) (A1) (B2) (A1) (B1) (A1) (A2) (B2)

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The electronic state of the initial guess is 2-B1.

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

Leave Link 401 at Sat Jun 15 12:05:06 2019, MaxMem= 1342177280 cpu: 43.3

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 2129573 IEndB= 2129573 NGot= 1342177280 MDV= 1340762408

LenX= 1340762408 LenY= 1340064348

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= 560000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 65426700.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.99D-15 for 4642.

Iteration 1 A\*A^-1 deviation from orthogonality is 5.14D-15 for 4664 1194.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.55D-15 for 4642.

Iteration 1 A^-1\*A deviation from orthogonality is 6.18D-08 for 2383 2362.

Iteration 2 A\*A^-1 deviation from unit magnitude is 3.11D-15 for 245.

Iteration 2 A\*A^-1 deviation from orthogonality is 3.74D-15 for 3610 617.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 306.

Iteration 2 A^-1\*A deviation from orthogonality is 5.19D-16 for 4642 1163.

E= -1732.64399178031

DIIS: error= 9.77D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1732.64399178031 IErMin= 1 ErrMin= 9.77D-02

ErrMax= 9.77D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.53D+00 BMatP= 4.53D+00

IDIUse=3 WtCom= 2.34D-02 WtEn= 9.77D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.029 Goal= None Shift= 0.000

Gap= 0.099 Goal= None Shift= 0.000

GapD= 0.029 DampG=0.250 DampE=0.250 DampFc=0.1250 IDamp=-1.

Damping current iteration by 1.25D-01

RMSDP=2.77D-03 MaxDP=9.23D-02 OVMax= 2.36D-01

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.46D-04 CP: 9.98D-01

E= -1732.82423888414 Delta-E= -0.180247103834 Rises=F Damp=T

DIIS: error= 6.95D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1732.82423888414 IErMin= 2 ErrMin= 6.95D-02

ErrMax= 6.95D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.61D+00 BMatP= 4.53D+00

IDIUse=3 WtCom= 3.05D-01 WtEn= 6.95D-01

Coeff-Com: -0.288D+01 0.388D+01

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

Coeff: -0.880D+00 0.188D+01

Gap= 0.031 Goal= None Shift= 0.000

Gap= 0.087 Goal= None Shift= 0.000

RMSDP=1.69D-03 MaxDP=6.00D-02 DE=-1.80D-01 OVMax= 6.64D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.03D-03 CP: 9.85D-01 3.00D+00

E= -1733.30236173797 Delta-E= -0.478122853827 Rises=F Damp=F

DIIS: error= 5.43D-02 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1733.30236173797 IErMin= 3 ErrMin= 5.43D-02

ErrMax= 5.43D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.05D+00 BMatP= 2.61D+00

IDIUse=3 WtCom= 4.57D-01 WtEn= 5.43D-01

EnCoef did 100 forward-backward iterations

Coeff-Com: 0.265D+01-0.281D+01 0.116D+01

Coeff-En: 0.124D+00 0.322D-02 0.872D+00

Coeff: 0.128D+01-0.128D+01 0.100D+01

Gap= 0.035 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=9.33D-04 MaxDP=3.49D-02 DE=-4.78D-01 OVMax= 7.21D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 5.17D-04 CP: 9.86D-01 3.00D+00 2.43D-01

E= -1733.46908384751 Delta-E= -0.166722109539 Rises=F Damp=F

DIIS: error= 2.21D-02 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1733.46908384751 IErMin= 4 ErrMin= 2.21D-02

ErrMax= 2.21D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.97D-01 BMatP= 1.05D+00

IDIUse=3 WtCom= 7.79D-01 WtEn= 2.21D-01

Coeff-Com: -0.900D+00 0.107D+01 0.938D-01 0.733D+00

Coeff-En: 0.000D+00 0.000D+00 0.116D+00 0.884D+00

Coeff: -0.701D+00 0.836D+00 0.987D-01 0.766D+00

Gap= 0.036 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=2.71D-04 MaxDP=1.10D-02 DE=-1.67D-01 OVMax= 4.17D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 8.75D-05 CP: 9.85D-01 3.00D+00 4.44D-01 7.04D-01

E= -1733.50429947889 Delta-E= -0.035215631382 Rises=F Damp=F

DIIS: error= 2.20D-03 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1733.50429947889 IErMin= 5 ErrMin= 2.20D-03

ErrMax= 2.20D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.10D-02 BMatP= 1.97D-01

IDIUse=3 WtCom= 9.78D-01 WtEn= 2.20D-02

Coeff-Com: -0.426D+00 0.497D+00 0.448D-01 0.456D+00 0.428D+00

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

Coeff: -0.416D+00 0.486D+00 0.438D-01 0.446D+00 0.441D+00

Gap= 0.036 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=4.86D-05 MaxDP=3.29D-03 DE=-3.52D-02 OVMax= 1.02D-02

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.01D-05 CP: 9.86D-01 3.00D+00 4.21D-01 7.46D-01 6.52D-01

E= -1733.50657532640 Delta-E= -0.002275847509 Rises=F Damp=F

DIIS: error= 2.75D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1733.50657532640 IErMin= 6 ErrMin= 2.75D-04

ErrMax= 2.75D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.30D-04 BMatP= 1.10D-02

IDIUse=3 WtCom= 9.97D-01 WtEn= 2.75D-03

Coeff-Com: -0.150D+00 0.172D+00 0.741D-03 0.126D+00 0.143D+00 0.708D+00

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

Coeff: -0.150D+00 0.171D+00 0.739D-03 0.126D+00 0.143D+00 0.709D+00

Gap= 0.037 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=1.18D-05 MaxDP=6.05D-04 DE=-2.28D-03 OVMax= 2.01D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 9.97D-06 CP: 9.85D-01 3.00D+00 4.26D-01 7.50D-01 6.68D-01

CP: 8.55D-01

E= -1733.50661278333 Delta-E= -0.000037456930 Rises=F Damp=F

DIIS: error= 1.71D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1733.50661278333 IErMin= 7 ErrMin= 1.71D-04

ErrMax= 1.71D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.88D-05 BMatP= 1.30D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.71D-03

Coeff-Com: -0.690D-02 0.683D-02-0.182D-02 0.169D-03 0.338D-02 0.392D+00

Coeff-Com: 0.607D+00

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

Coeff-En: 0.100D+01

Coeff: -0.689D-02 0.682D-02-0.182D-02 0.169D-03 0.337D-02 0.391D+00

Coeff: 0.607D+00

Gap= 0.037 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=6.08D-06 MaxDP=3.10D-04 DE=-3.75D-05 OVMax= 1.70D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 4.38D-06 CP: 9.85D-01 3.00D+00 4.25D-01 7.50D-01 6.87D-01

CP: 1.04D+00 9.15D-01

E= -1733.50663156900 Delta-E= -0.000018785676 Rises=F Damp=F

DIIS: error= 8.41D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1733.50663156900 IErMin= 8 ErrMin= 8.41D-05

ErrMax= 8.41D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.43D-06 BMatP= 4.88D-05

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

Coeff-Com: 0.591D-01-0.683D-01-0.650D-03-0.494D-01-0.555D-01-0.132D+00

Coeff-Com: 0.241D+00 0.101D+01

Coeff: 0.591D-01-0.683D-01-0.650D-03-0.494D-01-0.555D-01-0.132D+00

Coeff: 0.241D+00 0.101D+01

Gap= 0.037 Goal= None Shift= 0.000

Gap= 0.077 Goal= None Shift= 0.000

RMSDP=4.77D-06 MaxDP=3.24D-04 DE=-1.88D-05 OVMax= 1.51D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.68D-06 CP: 9.85D-01 3.00D+00 4.26D-01 7.51D-01 6.93D-01

CP: 1.14D+00 1.20D+00 1.33D+00

E= -1733.50663988797 Delta-E= -0.000008318965 Rises=F Damp=F

DIIS: error= 5.99D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1733.50663988797 IErMin= 9 ErrMin= 5.99D-05

ErrMax= 5.99D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.69D-06 BMatP= 8.43D-06

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

Coeff-Com: 0.213D-01-0.244D-01-0.994D-03-0.189D-01-0.200D-01-0.143D+00

Coeff-Com: 0.199D-01 0.436D+00 0.730D+00

Coeff: 0.213D-01-0.244D-01-0.994D-03-0.189D-01-0.200D-01-0.143D+00

Coeff: 0.199D-01 0.436D+00 0.730D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.077 Goal= None Shift= 0.000

RMSDP=2.13D-06 MaxDP=1.46D-04 DE=-8.32D-06 OVMax= 5.36D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.51D-06 CP: 9.85D-01 3.00D+00 4.26D-01 7.51D-01 6.95D-01

CP: 1.16D+00 1.29D+00 1.54D+00 1.22D+00

E= -1733.50664132355 Delta-E= -0.000001435585 Rises=F Damp=F

DIIS: error= 4.40D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1733.50664132355 IErMin=10 ErrMin= 4.40D-05

ErrMax= 4.40D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.58D-06 BMatP= 2.69D-06

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

Coeff-Com: -0.398D-02 0.480D-02-0.694D-03 0.223D-02 0.477D-02-0.687D-01

Coeff-Com: -0.636D-01-0.401D-01 0.555D+00 0.610D+00

Coeff: -0.398D-02 0.480D-02-0.694D-03 0.223D-02 0.477D-02-0.687D-01

Coeff: -0.636D-01-0.401D-01 0.555D+00 0.610D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.077 Goal= None Shift= 0.000

RMSDP=1.38D-06 MaxDP=8.20D-05 DE=-1.44D-06 OVMax= 3.38D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 7.32D-07 CP: 9.85D-01 3.00D+00 4.26D-01 7.51D-01 6.98D-01

CP: 1.18D+00 1.35D+00 1.67D+00 1.40D+00 7.77D-01

E= -1733.50664202688 Delta-E= -0.000000703321 Rises=F Damp=F

DIIS: error= 9.69D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1733.50664202688 IErMin=11 ErrMin= 9.69D-06

ErrMax= 9.69D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.88D-08 BMatP= 1.58D-06

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

Coeff-Com: -0.146D-02 0.168D-02 0.119D-03 0.133D-02 0.161D-02 0.537D-02

Coeff-Com: -0.101D-01-0.426D-01-0.229D-01 0.579D-01 0.101D+01

Coeff: -0.146D-02 0.168D-02 0.119D-03 0.133D-02 0.161D-02 0.537D-02

Coeff: -0.101D-01-0.426D-01-0.229D-01 0.579D-01 0.101D+01

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.077 Goal= None Shift= 0.000

RMSDP=5.74D-07 MaxDP=3.40D-05 DE=-7.03D-07 OVMax= 1.45D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 3.59D-07 CP: 9.85D-01 3.00D+00 4.26D-01 7.51D-01 6.98D-01

CP: 1.18D+00 1.37D+00 1.70D+00 1.47D+00 8.85D-01

CP: 1.31D+00

E= -1733.50664213589 Delta-E= -0.000000109015 Rises=F Damp=F

DIIS: error= 9.10D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1733.50664213589 IErMin=12 ErrMin= 9.10D-06

ErrMax= 9.10D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.11D-08 BMatP= 7.88D-08

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

Coeff-Com: -0.285D-04-0.216D-04 0.317D-03 0.580D-03 0.269D-03 0.219D-01

Coeff-Com: 0.803D-02-0.184D-01-0.161D+00-0.122D+00 0.627D+00 0.644D+00

Coeff: -0.285D-04-0.216D-04 0.317D-03 0.580D-03 0.269D-03 0.219D-01

Coeff: 0.803D-02-0.184D-01-0.161D+00-0.122D+00 0.627D+00 0.644D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.077 Goal= None Shift= 0.000

RMSDP=3.38D-07 MaxDP=1.94D-05 DE=-1.09D-07 OVMax= 8.40D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 2.09D-07 CP: 9.85D-01 3.00D+00 4.26D-01 7.51D-01 6.98D-01

CP: 1.18D+00 1.38D+00 1.72D+00 1.51D+00 9.13D-01

CP: 1.60D+00 9.56D-01

E= -1733.50664217836 Delta-E= -0.000000042468 Rises=F Damp=F

DIIS: error= 5.02D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1733.50664217836 IErMin=13 ErrMin= 5.02D-06

ErrMax= 5.02D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.39D-08 BMatP= 6.11D-08

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

Coeff-Com: 0.280D-03-0.350D-03 0.131D-03 0.129D-03 0.874D-04 0.929D-02

Coeff-Com: 0.650D-02 0.370D-02-0.678D-01-0.759D-01-0.114D+00 0.313D+00

Coeff-Com: 0.925D+00

Coeff: 0.280D-03-0.350D-03 0.131D-03 0.129D-03 0.874D-04 0.929D-02

Coeff: 0.650D-02 0.370D-02-0.678D-01-0.759D-01-0.114D+00 0.313D+00

Coeff: 0.925D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.077 Goal= None Shift= 0.000

RMSDP=2.53D-07 MaxDP=1.37D-05 DE=-4.25D-08 OVMax= 6.20D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 1.17D-07 CP: 9.85D-01 3.00D+00 4.26D-01 7.51D-01 6.98D-01

CP: 1.18D+00 1.38D+00 1.73D+00 1.54D+00 9.72D-01

CP: 1.73D+00 1.38D+00 9.80D-01

E= -1733.50664219252 Delta-E= -0.000000014164 Rises=F Damp=F

DIIS: error= 2.39D-06 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1733.50664219252 IErMin=14 ErrMin= 2.39D-06

ErrMax= 2.39D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.32D-09 BMatP= 1.39D-08

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

Coeff-Com: -0.101D-03 0.111D-03-0.178D-04 0.862D-04 0.658D-04 0.157D-02

Coeff-Com: 0.266D-02 0.441D-02-0.750D-02-0.232D-01-0.215D+00 0.532D-01

Coeff-Com: 0.604D+00 0.580D+00

Coeff: -0.101D-03 0.111D-03-0.178D-04 0.862D-04 0.658D-04 0.157D-02

Coeff: 0.266D-02 0.441D-02-0.750D-02-0.232D-01-0.215D+00 0.532D-01

Coeff: 0.604D+00 0.580D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.077 Goal= None Shift= 0.000

RMSDP=1.00D-07 MaxDP=5.23D-06 DE=-1.42D-08 OVMax= 2.44D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 4.12D-08 CP: 9.85D-01 3.00D+00 4.26D-01 7.51D-01 6.98D-01

CP: 1.18D+00 1.38D+00 1.73D+00 1.55D+00 9.84D-01

CP: 1.79D+00 1.41D+00 1.30D+00 8.70D-01

E= -1733.50664219525 Delta-E= -0.000000002729 Rises=F Damp=F

DIIS: error= 1.11D-06 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1733.50664219525 IErMin=15 ErrMin= 1.11D-06

ErrMax= 1.11D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.99D-10 BMatP= 6.32D-09

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

Coeff-Com: -0.293D-04 0.375D-04-0.548D-04-0.136D-03-0.251D-03-0.149D-02

Coeff-Com: 0.455D-03 0.225D-02 0.113D-01 0.241D-02-0.735D-01-0.370D-01

Coeff-Com: 0.779D-01 0.264D+00 0.754D+00

Coeff: -0.293D-04 0.375D-04-0.548D-04-0.136D-03-0.251D-03-0.149D-02

Coeff: 0.455D-03 0.225D-02 0.113D-01 0.241D-02-0.735D-01-0.370D-01

Coeff: 0.779D-01 0.264D+00 0.754D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.077 Goal= None Shift= 0.000

RMSDP=3.23D-08 MaxDP=1.57D-06 DE=-2.73D-09 OVMax= 7.80D-06

Cycle 16 Pass 1 IDiag 1:

RMSU= 1.47D-08 CP: 9.85D-01 3.00D+00 4.26D-01 7.51D-01 6.98D-01

CP: 1.18D+00 1.38D+00 1.73D+00 1.55D+00 9.82D-01

CP: 1.80D+00 1.46D+00 1.31D+00 9.66D-01 8.91D-01

E= -1733.50664219564 Delta-E= -0.000000000387 Rises=F Damp=F

DIIS: error= 2.23D-07 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1733.50664219564 IErMin=16 ErrMin= 2.23D-07

ErrMax= 2.23D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.61D-11 BMatP= 6.99D-10

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

Coeff-Com: 0.159D-04-0.176D-04-0.139D-05-0.281D-04-0.606D-04-0.233D-03

Coeff-Com: -0.231D-03-0.182D-03 0.169D-02 0.204D-02 0.129D-01-0.751D-02

Coeff-Com: -0.459D-01-0.319D-01 0.441D-01 0.103D+01

Coeff: 0.159D-04-0.176D-04-0.139D-05-0.281D-04-0.606D-04-0.233D-03

Coeff: -0.231D-03-0.182D-03 0.169D-02 0.204D-02 0.129D-01-0.751D-02

Coeff: -0.459D-01-0.319D-01 0.441D-01 0.103D+01

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.077 Goal= None Shift= 0.000

RMSDP=8.30D-09 MaxDP=5.41D-07 DE=-3.87D-10 OVMax= 2.21D-06

Error on total polarization charges = 0.07601

SCF Done: E(UB3LYP) = -1733.50664220 A.U. after 16 cycles

NFock= 16 Conv=0.83D-08 -V/T= 1.9759

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7686 S= 0.5092

<L.S>= 0.000000000000E+00

KE= 1.776268588325D+03 PE=-1.287684941662D+04 EE= 5.002048870630D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -8.99

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7686, after 0.7503

Leave Link 502 at Sat Jun 15 12:08:41 2019, MaxMem= 1342177280 cpu: 2505.8

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

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

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Population analysis using the SCF density.

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Orbital symmetries:

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(A1) (B1) (A1) (A2) (B1) (B2) (A2) (B2) (B1) (A1)

(B2) (B1) (A2) (A1) (A2) (B2) (B1) (A2) (B2) (B1)

(A1) (A1) (A2) (A1) (A1) (B2) (B1) (A2) (A1) (A1)

(B2) (B1) (A2) (B2) (B1) (A2) (B2) (A2) (B1) (A1)

(B1) (A1) (A2) (B2) (A1) (B1) (B2) (A2) (A1) (B2)

(B1) (A2) (A1) (B2) (B1) (A2) (A1) (B1) (B2) (A2)

(A1) (B2) (A1) (B1)

The electronic state is 2-B1.

Alpha occ. eigenvalues -- -14.30525 -14.30525 -14.29820 -14.29820 -14.29820

Alpha occ. eigenvalues -- -14.29820 -14.29225 -14.29225 -10.23232 -10.23232

Alpha occ. eigenvalues -- -10.23232 -10.23232 -10.22408 -10.22408 -10.22407

Alpha occ. eigenvalues -- -10.22407 -10.17418 -10.17418 -10.17418 -10.17418

Alpha occ. eigenvalues -- -10.17352 -10.17352 -10.17352 -10.17352 -10.17296

Alpha occ. eigenvalues -- -10.17296 -10.17296 -10.17296 -10.17162 -10.17162

Alpha occ. eigenvalues -- -10.17162 -10.17162 -10.17157 -10.17157 -10.17157

Alpha occ. eigenvalues -- -10.17157 -10.16996 -10.16996 -10.16996 -10.16996

Alpha occ. eigenvalues -- -0.98554 -0.97207 -0.97188 -0.94562 -0.92337

Alpha occ. eigenvalues -- -0.88658 -0.88106 -0.85565 -0.84470 -0.84466

Alpha occ. eigenvalues -- -0.84433 -0.84120 -0.76405 -0.75170 -0.75084

Alpha occ. eigenvalues -- -0.74942 -0.74681 -0.74647 -0.74597 -0.74454

Alpha occ. eigenvalues -- -0.70887 -0.68334 -0.67696 -0.62800 -0.62443

Alpha occ. eigenvalues -- -0.61905 -0.61883 -0.61575 -0.60820 -0.58618

Alpha occ. eigenvalues -- -0.58496 -0.58033 -0.57689 -0.56802 -0.55790

Alpha occ. eigenvalues -- -0.55322 -0.55290 -0.54168 -0.53783 -0.53765

Alpha occ. eigenvalues -- -0.53591 -0.51736 -0.51435 -0.51351 -0.48668

Alpha occ. eigenvalues -- -0.48268 -0.47138 -0.47111 -0.46212 -0.45604

Alpha occ. eigenvalues -- -0.45603 -0.45322 -0.45167 -0.44783 -0.43312

Alpha occ. eigenvalues -- -0.43306 -0.43251 -0.43236 -0.43224 -0.43183

Alpha occ. eigenvalues -- -0.42103 -0.41586 -0.41443 -0.40875 -0.40750

Alpha occ. eigenvalues -- -0.37337 -0.37261 -0.36388 -0.36084 -0.36020

Alpha occ. eigenvalues -- -0.35849 -0.35824 -0.35706 -0.35304 -0.34572

Alpha occ. eigenvalues -- -0.33963 -0.33947 -0.33916 -0.33350 -0.31702

Alpha occ. eigenvalues -- -0.31639 -0.31058 -0.30961 -0.29514 -0.27472

Alpha occ. eigenvalues -- -0.26775 -0.26605 -0.25557 -0.25455 -0.25347

Alpha occ. eigenvalues -- -0.25096 -0.24998 -0.24857 -0.24215 -0.24187

Alpha occ. eigenvalues -- -0.24179 -0.23981 -0.18136 -0.12838

Alpha virt. eigenvalues -- -0.09075 -0.04368 -0.02738 -0.02272 -0.02042

Alpha virt. eigenvalues -- -0.01971 0.02573 0.02707 0.03025 0.03120

Alpha virt. eigenvalues -- 0.05262 0.05272 0.05748 0.05860 0.06066

Alpha virt. eigenvalues -- 0.07092 0.07094 0.07139 0.07248 0.07701

Alpha virt. eigenvalues -- 0.09079 0.09089 0.10026 0.10749 0.11580

Alpha virt. eigenvalues -- 0.11654 0.12050 0.12055 0.12674 0.12952

Alpha virt. eigenvalues -- 0.14608 0.15274 0.15399 0.16184 0.17439

Alpha virt. eigenvalues -- 0.18038 0.18097 0.18165 0.19539 0.20582

Alpha virt. eigenvalues -- 0.20728 0.21466 0.22040 0.22183 0.23029

Alpha virt. eigenvalues -- 0.24020 0.24034 0.24185 0.24527 0.25127

Alpha virt. eigenvalues -- 0.25381 0.25761 0.26879 0.27022 0.27435

Alpha virt. eigenvalues -- 0.27517 0.27962 0.28125 0.28790 0.28816

Alpha virt. eigenvalues -- 0.28866 0.29007 0.29377 0.30391 0.30635

Alpha virt. eigenvalues -- 0.30927 0.30988 0.32087 0.33257 0.33488

Alpha virt. eigenvalues -- 0.34153 0.34645 0.35647 0.35671 0.36252

Alpha virt. eigenvalues -- 0.36585 0.37065 0.37335 0.38037 0.38189

Alpha virt. eigenvalues -- 0.38790 0.39011 0.39036 0.39870 0.39875

Alpha virt. eigenvalues -- 0.40051 0.40750 0.40829 0.40891 0.40926

Alpha virt. eigenvalues -- 0.41338 0.41628 0.41951 0.42103 0.42411

Alpha virt. eigenvalues -- 0.42594 0.42792 0.42873 0.43013 0.43426

Alpha virt. eigenvalues -- 0.43454 0.43491 0.43608 0.43727 0.43748

Alpha virt. eigenvalues -- 0.43842 0.43979 0.44176 0.44289 0.45742

Alpha virt. eigenvalues -- 0.45886 0.47066 0.47074 0.47296 0.47364

Alpha virt. eigenvalues -- 0.47870 0.47882 0.47998 0.48327 0.48840

Alpha virt. eigenvalues -- 0.50266 0.50408 0.50510 0.51198 0.51511

Alpha virt. eigenvalues -- 0.51593 0.51904 0.51972 0.52261 0.52262

Alpha virt. eigenvalues -- 0.52478 0.53592 0.54370 0.54427 0.54684

Alpha virt. eigenvalues -- 0.55163 0.56160 0.56171 0.57060 0.58995

Alpha virt. eigenvalues -- 0.60189 0.60372 0.60736 0.60747 0.60836

Alpha virt. eigenvalues -- 0.60844 0.60927 0.61340 0.61362 0.61389

Alpha virt. eigenvalues -- 0.61870 0.62227 0.62334 0.63282 0.63350

Alpha virt. eigenvalues -- 0.63423 0.63470 0.63793 0.64831 0.65067

Alpha virt. eigenvalues -- 0.65205 0.65269 0.65270 0.66377 0.67156

Alpha virt. eigenvalues -- 0.67332 0.67394 0.67984 0.68042 0.69849

Alpha virt. eigenvalues -- 0.70296 0.70338 0.70723 0.70906 0.71084

Alpha virt. eigenvalues -- 0.71412 0.72177 0.72548 0.73728 0.73966

Alpha virt. eigenvalues -- 0.74176 0.74537 0.75002 0.75269 0.76619

Alpha virt. eigenvalues -- 0.77481 0.77546 0.77731 0.77827 0.77893

Alpha virt. eigenvalues -- 0.78672 0.78803 0.79628 0.80046 0.80048

Alpha virt. eigenvalues -- 0.80171 0.80403 0.80817 0.81840 0.82215

Alpha virt. eigenvalues -- 0.82275 0.82413 0.83415 0.83692 0.84471

Alpha virt. eigenvalues -- 0.84594 0.86670 0.86908 0.87068 0.87321

Alpha virt. eigenvalues -- 0.87464 0.88697 0.89175 0.89308 0.89868

Alpha virt. eigenvalues -- 0.90573 0.91110 0.91325 0.91585 0.91804

Alpha virt. eigenvalues -- 0.92504 0.92769 0.93088 0.94418 0.94991

Alpha virt. eigenvalues -- 0.96477 0.98045 0.99557 0.99650 0.99710

Alpha virt. eigenvalues -- 1.00203 1.00408 1.00445 1.00586 1.01087

Alpha virt. eigenvalues -- 1.02558 1.02594 1.02785 1.03584 1.03663

Alpha virt. eigenvalues -- 1.06237 1.06338 1.06519 1.07387 1.10940

Alpha virt. eigenvalues -- 1.11033 1.11309 1.11412 1.11528 1.12042

Alpha virt. eigenvalues -- 1.12279 1.12371 1.12798 1.14153 1.14421

Alpha virt. eigenvalues -- 1.14873 1.14928 1.15086 1.15490 1.16144

Alpha virt. eigenvalues -- 1.17152 1.19056 1.19906 1.21046 1.21075

Alpha virt. eigenvalues -- 1.21230 1.21304 1.21443 1.21538 1.21551

Alpha virt. eigenvalues -- 1.21566 1.23396 1.23559 1.25968 1.26209

Alpha virt. eigenvalues -- 1.26308 1.26649 1.27505 1.27551 1.27712

Alpha virt. eigenvalues -- 1.28530 1.29236 1.29629 1.30094 1.32438

Alpha virt. eigenvalues -- 1.34529 1.34794 1.34802 1.35346 1.35586

Alpha virt. eigenvalues -- 1.36260 1.39038 1.39787 1.42030 1.42271

Alpha virt. eigenvalues -- 1.42772 1.43173 1.43556 1.43588 1.45564

Alpha virt. eigenvalues -- 1.45699 1.45741 1.45806 1.45829 1.45870

Alpha virt. eigenvalues -- 1.48835 1.50248 1.51562 1.51652 1.52220

Alpha virt. eigenvalues -- 1.53132 1.53384 1.53454 1.53655 1.53656

Alpha virt. eigenvalues -- 1.54019 1.54116 1.55466 1.56194 1.58310

Alpha virt. eigenvalues -- 1.58311 1.60193 1.62734 1.62773 1.63163

Alpha virt. eigenvalues -- 1.63369 1.64063 1.65121 1.66100 1.66298

Alpha virt. eigenvalues -- 1.67024 1.67871 1.68747 1.69007 1.72531

Alpha virt. eigenvalues -- 1.72553 1.72898 1.74395 1.74496 1.74683

Alpha virt. eigenvalues -- 1.74879 1.75241 1.76000 1.76017 1.76035

Alpha virt. eigenvalues -- 1.81440 1.81563 1.81634 1.81661 1.82199

Alpha virt. eigenvalues -- 1.82817 1.83092 1.83458 1.83557 1.83870

Alpha virt. eigenvalues -- 1.84675 1.84929 1.85201 1.86879 1.87034

Alpha virt. eigenvalues -- 1.87391 1.89453 1.90182 1.91044 1.91170

Alpha virt. eigenvalues -- 1.91195 1.91256 1.91338 1.91524 1.91557

Alpha virt. eigenvalues -- 1.91560 1.91768 1.92285 1.92668 1.92784

Alpha virt. eigenvalues -- 1.93152 1.93379 1.94147 1.95010 1.95406

Alpha virt. eigenvalues -- 1.95792 1.96681 1.99206 1.99424 1.99611

Alpha virt. eigenvalues -- 2.00344 2.01560 2.02995 2.03032 2.03533

Alpha virt. eigenvalues -- 2.04220 2.05039 2.05903 2.06001 2.08373

Alpha virt. eigenvalues -- 2.12068 2.14249 2.14271 2.16431 2.16434

Alpha virt. eigenvalues -- 2.18582 2.19910 2.22233 2.23280 2.23817

Alpha virt. eigenvalues -- 2.24017 2.24422 2.25031 2.25499 2.25875

Alpha virt. eigenvalues -- 2.26719 2.27145 2.27625 2.27702 2.28095

Alpha virt. eigenvalues -- 2.28337 2.28409 2.28763 2.29129 2.30528

Alpha virt. eigenvalues -- 2.30711 2.30741 2.30921 2.33027 2.33327

Alpha virt. eigenvalues -- 2.33347 2.33906 2.37568 2.38931 2.39193

Alpha virt. eigenvalues -- 2.39852 2.40109 2.40140 2.41142 2.41869

Alpha virt. eigenvalues -- 2.43778 2.43888 2.44520 2.45763 2.46644

Alpha virt. eigenvalues -- 2.49401 2.49475 2.52412 2.53054 2.53854

Alpha virt. eigenvalues -- 2.53959 2.55143 2.55829 2.56626 2.56830

Alpha virt. eigenvalues -- 2.57875 2.58168 2.58521 2.58611 2.59728

Alpha virt. eigenvalues -- 2.61666 2.64692 2.65143 2.65461 2.66145

Alpha virt. eigenvalues -- 2.66193 2.66629 2.68772 2.68812 2.69277

Alpha virt. eigenvalues -- 2.69325 2.70639 2.73535 2.74530 2.74569

Alpha virt. eigenvalues -- 2.74774 2.75071 2.75221 2.75379 2.76067

Alpha virt. eigenvalues -- 2.77573 2.77704 2.77820 2.78860 2.79579

Alpha virt. eigenvalues -- 2.79828 2.80060 2.82460 2.82700 2.83017

Alpha virt. eigenvalues -- 2.83068 2.83136 2.84339 2.85095 2.86049

Alpha virt. eigenvalues -- 2.86623 2.88580 2.88599 2.88791 2.89072

Alpha virt. eigenvalues -- 2.92160 2.92274 2.92306 2.92340 2.92548

Alpha virt. eigenvalues -- 2.97713 2.98022 3.00482 3.04212 3.05247

Alpha virt. eigenvalues -- 3.05262 3.05527 3.07987 3.08663 3.09779

Alpha virt. eigenvalues -- 3.15857 3.16691 3.16717 3.16931 3.17734

Alpha virt. eigenvalues -- 3.18925 3.19766 3.19900 3.20245 3.21733

Alpha virt. eigenvalues -- 3.22752 3.23113 3.23724 3.26280 3.26527

Alpha virt. eigenvalues -- 3.26894 3.26918 3.27653 3.27764 3.27963

Alpha virt. eigenvalues -- 3.28718 3.30540 3.30945 3.31133 3.31203

Alpha virt. eigenvalues -- 3.31348 3.33234 3.33351 3.36340 3.38034

Alpha virt. eigenvalues -- 3.40171 3.40219 3.41706 3.46489 3.47349

Alpha virt. eigenvalues -- 3.47441 3.47764 3.48220 3.48370 3.48477

Alpha virt. eigenvalues -- 3.49934 3.56774 3.61714 3.62188 3.64523

Alpha virt. eigenvalues -- 3.64534 3.64637 3.65127 3.72632 3.72809

Alpha virt. eigenvalues -- 3.73470 3.74490 3.75895 3.76763 3.77372

Alpha virt. eigenvalues -- 3.77425 3.83116 3.84344 3.84604 3.84889

Alpha virt. eigenvalues -- 3.88004 3.89079 3.90477 3.90819 3.91716

Alpha virt. eigenvalues -- 3.95850 3.96582 3.96608 3.97499 4.10987

Alpha virt. eigenvalues -- 4.12070 4.12664 4.18330 4.18729 4.18842

Alpha virt. eigenvalues -- 4.20888 4.23676 4.35161 4.40306 4.41180

Alpha virt. eigenvalues -- 4.41337 4.47111 4.53323 4.55348 4.55433

Alpha virt. eigenvalues -- 4.78756 4.78915 4.78915 4.79230 5.12571

Alpha virt. eigenvalues -- 5.13380 5.13995 5.16933 5.21234 5.35161

Alpha virt. eigenvalues -- 5.37413 5.52616 7.85697 7.85834 7.86332

Alpha virt. eigenvalues -- 7.92286 8.15793 11.13325 23.28468 23.31532

Alpha virt. eigenvalues -- 23.31544 23.33298 23.76713 23.78439 23.78640

Alpha virt. eigenvalues -- 23.78669 23.78901 23.78982 23.79188 23.80795

Alpha virt. eigenvalues -- 23.88450 23.88732 23.89576 23.89753 23.90880

Alpha virt. eigenvalues -- 23.90949 23.91002 23.91472 24.02460 24.02722

Alpha virt. eigenvalues -- 24.02781 24.03331 24.04973 24.04985 24.05032

Alpha virt. eigenvalues -- 24.05107 24.12786 24.12931 24.12951 24.13292

Alpha virt. eigenvalues -- 35.57673 35.61108 35.61594 35.62364 35.69512

Alpha virt. eigenvalues -- 35.70229 35.70274 35.70408

Beta occ. eigenvalues -- -14.30644 -14.30643 -14.29765 -14.29765 -14.29765

Beta occ. eigenvalues -- -14.29764 -14.28890 -14.28890 -10.23269 -10.23269

Beta occ. eigenvalues -- -10.23268 -10.23268 -10.22175 -10.22175 -10.22174

Beta occ. eigenvalues -- -10.22174 -10.17449 -10.17449 -10.17449 -10.17449

Beta occ. eigenvalues -- -10.17352 -10.17352 -10.17352 -10.17351 -10.17285

Beta occ. eigenvalues -- -10.17285 -10.17285 -10.17285 -10.17178 -10.17178

Beta occ. eigenvalues -- -10.17178 -10.17178 -10.17092 -10.17092 -10.17092

Beta occ. eigenvalues -- -10.17092 -10.16937 -10.16937 -10.16937 -10.16937

Beta occ. eigenvalues -- -0.98331 -0.97014 -0.96937 -0.94374 -0.92077

Beta occ. eigenvalues -- -0.88639 -0.87650 -0.85411 -0.84414 -0.84409

Beta occ. eigenvalues -- -0.84348 -0.83949 -0.76260 -0.75047 -0.75038

Beta occ. eigenvalues -- -0.74854 -0.74627 -0.74559 -0.74512 -0.74361

Beta occ. eigenvalues -- -0.70674 -0.67905 -0.67661 -0.62680 -0.62377

Beta occ. eigenvalues -- -0.61848 -0.61829 -0.61424 -0.60735 -0.58545

Beta occ. eigenvalues -- -0.58422 -0.57928 -0.57618 -0.56788 -0.55775

Beta occ. eigenvalues -- -0.55283 -0.55282 -0.54114 -0.53731 -0.53688

Beta occ. eigenvalues -- -0.53515 -0.51611 -0.51356 -0.51313 -0.48580

Beta occ. eigenvalues -- -0.48164 -0.47088 -0.46993 -0.46177 -0.45567

Beta occ. eigenvalues -- -0.45564 -0.45252 -0.45131 -0.44233 -0.43279

Beta occ. eigenvalues -- -0.43220 -0.43207 -0.43176 -0.42762 -0.42703

Beta occ. eigenvalues -- -0.42060 -0.41534 -0.41413 -0.40835 -0.40341

Beta occ. eigenvalues -- -0.37279 -0.36498 -0.36348 -0.36038 -0.35984

Beta occ. eigenvalues -- -0.35606 -0.35508 -0.35507 -0.35252 -0.34550

Beta occ. eigenvalues -- -0.33927 -0.33894 -0.33651 -0.33322 -0.31547

Beta occ. eigenvalues -- -0.31524 -0.30855 -0.29955 -0.29354 -0.27132

Beta occ. eigenvalues -- -0.26656 -0.26423 -0.25382 -0.25262 -0.25017

Beta occ. eigenvalues -- -0.24996 -0.24848 -0.24621 -0.23955 -0.23775

Beta occ. eigenvalues -- -0.23733 -0.23226 -0.16922

Beta virt. eigenvalues -- -0.09192 -0.08717 -0.03466 -0.02399 -0.02088

Beta virt. eigenvalues -- -0.01807 -0.01752 0.02924 0.03173 0.03206

Beta virt. eigenvalues -- 0.03314 0.05299 0.05302 0.05879 0.06432

Beta virt. eigenvalues -- 0.06693 0.07108 0.07110 0.07146 0.07285

Beta virt. eigenvalues -- 0.07708 0.09082 0.09101 0.10041 0.10756

Beta virt. eigenvalues -- 0.12048 0.12065 0.12335 0.12341 0.12691

Beta virt. eigenvalues -- 0.13479 0.14617 0.15298 0.15402 0.16193

Beta virt. eigenvalues -- 0.17702 0.18352 0.18462 0.18491 0.19680

Beta virt. eigenvalues -- 0.20803 0.20830 0.21477 0.22157 0.22439

Beta virt. eigenvalues -- 0.23271 0.24073 0.24098 0.24452 0.24671

Beta virt. eigenvalues -- 0.25179 0.25457 0.25804 0.26964 0.27136

Beta virt. eigenvalues -- 0.27495 0.27570 0.27999 0.28253 0.28839

Beta virt. eigenvalues -- 0.28871 0.28926 0.29081 0.29418 0.30560

Beta virt. eigenvalues -- 0.30703 0.31010 0.31011 0.32302 0.33327

Beta virt. eigenvalues -- 0.33620 0.34241 0.34668 0.35719 0.35773

Beta virt. eigenvalues -- 0.36413 0.36697 0.37336 0.37402 0.38093

Beta virt. eigenvalues -- 0.38282 0.38864 0.39082 0.39157 0.39946

Beta virt. eigenvalues -- 0.40021 0.40113 0.40836 0.40942 0.40942

Beta virt. eigenvalues -- 0.40944 0.41566 0.41716 0.42063 0.42240

Beta virt. eigenvalues -- 0.42494 0.42652 0.42891 0.42976 0.43056

Beta virt. eigenvalues -- 0.43504 0.43523 0.43534 0.43742 0.43768

Beta virt. eigenvalues -- 0.43928 0.43973 0.44150 0.44218 0.44388

Beta virt. eigenvalues -- 0.45812 0.45939 0.47231 0.47234 0.47319

Beta virt. eigenvalues -- 0.47435 0.47949 0.47971 0.48055 0.48407

Beta virt. eigenvalues -- 0.48904 0.50454 0.50516 0.50620 0.51351

Beta virt. eigenvalues -- 0.51540 0.51681 0.51987 0.52155 0.52381

Beta virt. eigenvalues -- 0.52393 0.52610 0.53660 0.54474 0.54493

Beta virt. eigenvalues -- 0.54807 0.55258 0.56247 0.56292 0.57176

Beta virt. eigenvalues -- 0.59143 0.60286 0.60469 0.60753 0.60789

Beta virt. eigenvalues -- 0.60890 0.60898 0.60964 0.61365 0.61392

Beta virt. eigenvalues -- 0.61656 0.62049 0.62285 0.62394 0.63336

Beta virt. eigenvalues -- 0.63418 0.63535 0.63547 0.63864 0.64887

Beta virt. eigenvalues -- 0.65108 0.65262 0.65327 0.65346 0.66439

Beta virt. eigenvalues -- 0.67243 0.67457 0.67473 0.68096 0.68106

Beta virt. eigenvalues -- 0.69948 0.70388 0.70436 0.70784 0.71131

Beta virt. eigenvalues -- 0.71164 0.71608 0.72349 0.72609 0.73797

Beta virt. eigenvalues -- 0.74011 0.74275 0.74578 0.75126 0.75304

Beta virt. eigenvalues -- 0.76799 0.77502 0.77608 0.77744 0.77911

Beta virt. eigenvalues -- 0.77965 0.78782 0.79155 0.79754 0.80051

Beta virt. eigenvalues -- 0.80212 0.80247 0.80605 0.80970 0.82085

Beta virt. eigenvalues -- 0.82309 0.82350 0.82458 0.83468 0.83719

Beta virt. eigenvalues -- 0.84522 0.84626 0.86716 0.87102 0.87188

Beta virt. eigenvalues -- 0.87447 0.87479 0.88735 0.89251 0.89351

Beta virt. eigenvalues -- 0.89920 0.90625 0.91173 0.91343 0.91668

Beta virt. eigenvalues -- 0.91840 0.92567 0.92925 0.93173 0.94460

Beta virt. eigenvalues -- 0.95067 0.96528 0.98194 0.99622 0.99707

Beta virt. eigenvalues -- 0.99820 1.00321 1.00495 1.00495 1.00655

Beta virt. eigenvalues -- 1.01171 1.02620 1.02633 1.02806 1.03703

Beta virt. eigenvalues -- 1.03725 1.06399 1.06499 1.06693 1.07457

Beta virt. eigenvalues -- 1.11051 1.11070 1.11457 1.11599 1.11767

Beta virt. eigenvalues -- 1.12269 1.12416 1.12536 1.12859 1.14276

Beta virt. eigenvalues -- 1.14532 1.15032 1.15054 1.15190 1.15665

Beta virt. eigenvalues -- 1.16302 1.17255 1.19432 1.19977 1.21157

Beta virt. eigenvalues -- 1.21226 1.21286 1.21419 1.21497 1.21611

Beta virt. eigenvalues -- 1.21619 1.21664 1.23453 1.23656 1.26013

Beta virt. eigenvalues -- 1.26355 1.26600 1.26717 1.27548 1.27606

Beta virt. eigenvalues -- 1.27789 1.28597 1.29273 1.29708 1.30289

Beta virt. eigenvalues -- 1.32522 1.34657 1.34958 1.34967 1.35477

Beta virt. eigenvalues -- 1.35718 1.36383 1.39332 1.39989 1.42288

Beta virt. eigenvalues -- 1.42449 1.43074 1.43201 1.43600 1.43700

Beta virt. eigenvalues -- 1.45556 1.45730 1.45784 1.45818 1.45858

Beta virt. eigenvalues -- 1.46070 1.48914 1.50294 1.51579 1.51686

Beta virt. eigenvalues -- 1.52285 1.53232 1.53608 1.53629 1.53838

Beta virt. eigenvalues -- 1.53887 1.54084 1.54234 1.55547 1.56329

Beta virt. eigenvalues -- 1.58407 1.58478 1.60353 1.62905 1.63029

Beta virt. eigenvalues -- 1.63297 1.63566 1.64180 1.65194 1.66180

Beta virt. eigenvalues -- 1.66429 1.67114 1.68025 1.68899 1.69091

Beta virt. eigenvalues -- 1.72645 1.72718 1.72980 1.74455 1.74562

Beta virt. eigenvalues -- 1.74781 1.74885 1.75335 1.76035 1.76084

Beta virt. eigenvalues -- 1.76128 1.81557 1.81689 1.81699 1.81740

Beta virt. eigenvalues -- 1.82307 1.82951 1.83251 1.83532 1.83577

Beta virt. eigenvalues -- 1.83931 1.84752 1.85021 1.85401 1.86945

Beta virt. eigenvalues -- 1.87163 1.87523 1.89511 1.90340 1.91157

Beta virt. eigenvalues -- 1.91252 1.91298 1.91335 1.91466 1.91628

Beta virt. eigenvalues -- 1.91643 1.91682 1.91908 1.92313 1.92789

Beta virt. eigenvalues -- 1.92814 1.93292 1.93429 1.94193 1.95062

Beta virt. eigenvalues -- 1.95453 1.95864 1.96733 1.99390 1.99504

Beta virt. eigenvalues -- 1.99809 2.00537 2.01711 2.03166 2.03269

Beta virt. eigenvalues -- 2.03741 2.04553 2.05258 2.06171 2.06331

Beta virt. eigenvalues -- 2.08583 2.12169 2.14593 2.14597 2.16425

Beta virt. eigenvalues -- 2.16616 2.18675 2.20053 2.22492 2.23492

Beta virt. eigenvalues -- 2.23953 2.24159 2.24466 2.25153 2.25547

Beta virt. eigenvalues -- 2.25907 2.26741 2.27197 2.27677 2.27758

Beta virt. eigenvalues -- 2.28195 2.28500 2.28609 2.28823 2.29324

Beta virt. eigenvalues -- 2.30556 2.30736 2.30773 2.30959 2.33058

Beta virt. eigenvalues -- 2.33340 2.33426 2.33955 2.37782 2.38966

Beta virt. eigenvalues -- 2.39224 2.40135 2.40191 2.40275 2.41316

Beta virt. eigenvalues -- 2.42093 2.43934 2.44257 2.44839 2.45907

Beta virt. eigenvalues -- 2.46940 2.49480 2.49679 2.52714 2.53186

Beta virt. eigenvalues -- 2.54022 2.54076 2.55282 2.55976 2.56869

Beta virt. eigenvalues -- 2.56876 2.57916 2.58271 2.58547 2.58830

Beta virt. eigenvalues -- 2.59791 2.61892 2.64954 2.65430 2.65549

Beta virt. eigenvalues -- 2.66326 2.66514 2.66724 2.68877 2.69050

Beta virt. eigenvalues -- 2.69425 2.69595 2.70799 2.73690 2.74842

Beta virt. eigenvalues -- 2.74871 2.74918 2.75226 2.75365 2.75582

Beta virt. eigenvalues -- 2.76119 2.77737 2.77739 2.77869 2.78967

Beta virt. eigenvalues -- 2.79891 2.80103 2.80235 2.82743 2.82840

Beta virt. eigenvalues -- 2.83121 2.83314 2.83355 2.84384 2.85158

Beta virt. eigenvalues -- 2.86213 2.86668 2.88663 2.88781 2.89063

Beta virt. eigenvalues -- 2.89145 2.92235 2.92339 2.92398 2.92536

Beta virt. eigenvalues -- 2.92893 2.97876 2.98497 3.00731 3.04317

Beta virt. eigenvalues -- 3.05394 3.05401 3.05600 3.08232 3.08737

Beta virt. eigenvalues -- 3.09838 3.15879 3.16714 3.16741 3.16955

Beta virt. eigenvalues -- 3.17793 3.19044 3.19915 3.19924 3.20296

Beta virt. eigenvalues -- 3.21782 3.22785 3.23155 3.23765 3.26342

Beta virt. eigenvalues -- 3.26555 3.26932 3.26965 3.27674 3.27784

Beta virt. eigenvalues -- 3.28004 3.28773 3.30564 3.30974 3.31168

Beta virt. eigenvalues -- 3.31237 3.31384 3.33255 3.33388 3.36375

Beta virt. eigenvalues -- 3.38064 3.40201 3.40245 3.41729 3.46521

Beta virt. eigenvalues -- 3.47381 3.47474 3.47794 3.48249 3.48400

Beta virt. eigenvalues -- 3.48510 3.49967 3.56872 3.61805 3.62278

Beta virt. eigenvalues -- 3.64554 3.64560 3.64664 3.65155 3.72707

Beta virt. eigenvalues -- 3.72871 3.73534 3.74574 3.75948 3.76846

Beta virt. eigenvalues -- 3.77461 3.77537 3.83538 3.84505 3.84969

Beta virt. eigenvalues -- 3.85261 3.88299 3.89643 3.90829 3.91278

Beta virt. eigenvalues -- 3.92076 3.95893 3.96629 3.96649 3.97543

Beta virt. eigenvalues -- 4.11053 4.12069 4.12822 4.18411 4.18806

Beta virt. eigenvalues -- 4.18934 4.20982 4.23761 4.35283 4.40481

Beta virt. eigenvalues -- 4.41340 4.41472 4.47237 4.53410 4.55469

Beta virt. eigenvalues -- 4.55511 4.78803 4.78964 4.78964 4.79281

Beta virt. eigenvalues -- 5.12748 5.13508 5.14143 5.17075 5.21421

Beta virt. eigenvalues -- 5.35355 5.37572 5.52794 7.85701 7.85863

Beta virt. eigenvalues -- 7.86331 7.92290 8.15797 11.13335 23.28491

Beta virt. eigenvalues -- 23.31553 23.31566 23.33319 23.76798 23.78454

Beta virt. eigenvalues -- 23.78655 23.78688 23.78915 23.79040 23.79289

Beta virt. eigenvalues -- 23.80874 23.88481 23.88781 23.89687 23.89776

Beta virt. eigenvalues -- 23.90975 23.91010 23.91119 23.91624 24.02487

Beta virt. eigenvalues -- 24.02747 24.02808 24.03355 24.04989 24.05001

Beta virt. eigenvalues -- 24.05050 24.05124 24.12803 24.12949 24.12968

Beta virt. eigenvalues -- 24.13310 35.57755 35.61211 35.61630 35.62423

Beta virt. eigenvalues -- 35.69601 35.70309 35.70392 35.70538

Condensed to atoms (all electrons):

Atomic-Atomic Spin Densities.

Mulliken charges and spin densities:

1 2

1 C 0.361610 -0.019012

2 N -0.667390 0.023010

3 C 0.318955 0.142538

4 C -0.052492 -0.022724

5 C -0.078615 0.048300

6 N -0.397137 -0.063862

7 C 0.318955 0.142538

8 N -0.667390 0.023010

9 C 0.361610 -0.019012

10 C -0.078615 0.048300

11 C -0.052492 -0.022724

12 N -0.446002 0.151884

13 C -0.078615 0.048300

14 C -0.052492 -0.022724

15 C 0.318955 0.142538

16 N -0.667390 0.023010

17 C 0.361610 -0.019012

18 N -0.397137 -0.063862

19 N -0.667390 0.023010

20 C 0.318955 0.142538

21 C -0.052492 -0.022724

22 C -0.078615 0.048300

23 C 0.361610 -0.019012

24 N -0.446002 0.151884

25 Zn 1.363862 -0.002656

26 C -0.224037 -0.023967

27 C -0.241531 0.044804

28 C -0.233396 -0.019027

29 C -0.231489 0.035242

30 C -0.224037 -0.023967

31 C -0.241531 0.044804

32 C -0.233396 -0.019027

33 C -0.231489 0.035242

34 C -0.231489 0.035242

35 C -0.233396 -0.019027

36 C -0.241531 0.044804

37 C -0.224037 -0.023967

38 C -0.224037 -0.023967

39 C -0.241531 0.044804

40 C -0.233396 -0.019027

41 C -0.231489 0.035242

42 H 0.216510 0.000796

43 H 0.216567 -0.001601

44 H 0.216510 0.000796

45 H 0.216567 -0.001601

46 H 0.216567 -0.001601

47 H 0.216510 0.000796

48 H 0.216510 0.000796

49 H 0.216567 -0.001601

50 H 0.223291 0.000796

51 H 0.222620 -0.002502

52 H 0.223291 0.000796

53 H 0.222620 -0.002502

54 H 0.222620 -0.002502

55 H 0.223291 0.000796

56 H 0.223291 0.000796

57 H 0.222620 -0.002502

Sum of Mulliken charges = -1.00000 1.00000

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

1 2

1 C 0.361610 -0.019012

2 N -0.667390 0.023010

3 C 0.318955 0.142538

4 C -0.052492 -0.022724

5 C -0.078615 0.048300

6 N -0.397137 -0.063862

7 C 0.318955 0.142538

8 N -0.667390 0.023010

9 C 0.361610 -0.019012

10 C -0.078615 0.048300

11 C -0.052492 -0.022724

12 N -0.446002 0.151884

13 C -0.078615 0.048300

14 C -0.052492 -0.022724

15 C 0.318955 0.142538

16 N -0.667390 0.023010

17 C 0.361610 -0.019012

18 N -0.397137 -0.063862

19 N -0.667390 0.023010

20 C 0.318955 0.142538

21 C -0.052492 -0.022724

22 C -0.078615 0.048300

23 C 0.361610 -0.019012

24 N -0.446002 0.151884

25 Zn 1.363862 -0.002656

26 C -0.007527 -0.023171

27 C -0.018911 0.042302

28 C -0.010105 -0.018231

29 C -0.014922 0.033641

30 C -0.007527 -0.023171

31 C -0.018911 0.042302

32 C -0.010105 -0.018231

33 C -0.014922 0.033641

34 C -0.014922 0.033641

35 C -0.010105 -0.018231

36 C -0.018911 0.042302

37 C -0.007527 -0.023171

38 C -0.007527 -0.023171

39 C -0.018911 0.042302

40 C -0.010105 -0.018231

41 C -0.014922 0.033641

Electronic spatial extent (au): <R\*\*2>= 22467.6999

Charge= -1.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 0.0000 Y= 0.0000 Z= 2.1838 Tot= 2.1838

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

XX= -260.5370 YY= -257.5731 ZZ= -248.4180

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

XX= -5.0276 YY= -2.0638 ZZ= 7.0914

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

XXX= 0.0000 YYY= 0.0000 ZZZ= 26.7745 XYY= 0.0000

XXY= 0.0000 XXZ= -1.1024 XZZ= 0.0000 YZZ= 0.0000

YYZ= -1.0627 XYZ= 0.0000

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

XXXX= -14826.3820 YYYY= -14709.6939 ZZZZ= -286.4298 XXXY= 0.0000

XXXZ= 0.0000 YYYX= 0.0000 YYYZ= 0.0000 ZZZX= 0.0000

ZZZY= 0.0000 XXYY= -4718.9618 XXZZ= -2979.7899 YYZZ= -2975.5466

XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= 0.0000

N-N= 4.365025315469D+03 E-N=-1.287684939939D+04 KE= 1.776268588325D+03

Symmetry A1 KE= 5.097570824818D+02

Symmetry A2 KE= 3.905693050255D+02

Symmetry B1 KE= 4.387319917699D+02

Symmetry B2 KE= 4.372102090481D+02

Isotropic Fermi Contact Couplings

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

1 C(13) -0.00735 -8.26118 -2.94779 -2.75563

2 N(14) 0.00062 0.19944 0.07116 0.06653

3 C(13) 0.01069 12.01510 4.28729 4.00781

4 C(13) -0.00696 -7.81906 -2.79003 -2.60816

5 C(13) 0.00327 3.68137 1.31361 1.22797

6 N(14) -0.01147 -3.70538 -1.32217 -1.23598

7 C(13) 0.01069 12.01510 4.28729 4.00781

8 N(14) 0.00062 0.19944 0.07116 0.06653

9 C(13) -0.00735 -8.26118 -2.94779 -2.75563

10 C(13) 0.00327 3.68137 1.31361 1.22797

11 C(13) -0.00696 -7.81906 -2.79003 -2.60816

12 N(14) 0.01794 5.79603 2.06817 1.93335

13 C(13) 0.00327 3.68137 1.31361 1.22797

14 C(13) -0.00696 -7.81906 -2.79003 -2.60816

15 C(13) 0.01069 12.01510 4.28729 4.00781

16 N(14) 0.00062 0.19944 0.07116 0.06653

17 C(13) -0.00735 -8.26118 -2.94779 -2.75563

18 N(14) -0.01147 -3.70538 -1.32217 -1.23598

19 N(14) 0.00062 0.19944 0.07116 0.06653

20 C(13) 0.01069 12.01510 4.28729 4.00781

21 C(13) -0.00696 -7.81906 -2.79003 -2.60816

22 C(13) 0.00327 3.68137 1.31361 1.22797

23 C(13) -0.00735 -8.26118 -2.94779 -2.75563

24 N(14) 0.01794 5.79603 2.06817 1.93335

25 Zn(67) 0.00000 0.00000 0.00000 0.00000

26 C(13) -0.00348 -3.90959 -1.39504 -1.30410

27 C(13) 0.00312 3.50870 1.25199 1.17037

28 C(13) -0.00279 -3.13936 -1.12020 -1.04718

29 C(13) 0.00227 2.55705 0.91242 0.85294

30 C(13) -0.00348 -3.90959 -1.39504 -1.30410

31 C(13) 0.00312 3.50870 1.25199 1.17037

32 C(13) -0.00279 -3.13936 -1.12020 -1.04718

33 C(13) 0.00227 2.55705 0.91242 0.85294

34 C(13) 0.00227 2.55705 0.91242 0.85294

35 C(13) -0.00279 -3.13936 -1.12020 -1.04718

36 C(13) 0.00312 3.50870 1.25199 1.17037

37 C(13) -0.00348 -3.90959 -1.39504 -1.30410

38 C(13) -0.00348 -3.90959 -1.39504 -1.30410

39 C(13) 0.00312 3.50870 1.25199 1.17037

40 C(13) -0.00279 -3.13936 -1.12020 -1.04718

41 C(13) 0.00227 2.55705 0.91242 0.85294

42 H(1) 0.00027 1.22897 0.43853 0.40994

43 H(1) -0.00050 -2.22415 -0.79363 -0.74190

44 H(1) 0.00027 1.22897 0.43853 0.40994

45 H(1) -0.00050 -2.22415 -0.79363 -0.74190

46 H(1) -0.00050 -2.22415 -0.79363 -0.74190

47 H(1) 0.00027 1.22897 0.43853 0.40994

48 H(1) 0.00027 1.22897 0.43853 0.40994

49 H(1) -0.00050 -2.22415 -0.79363 -0.74190

50 H(1) 0.00020 0.90404 0.32258 0.30155

51 H(1) -0.00064 -2.87668 -1.02647 -0.95956

52 H(1) 0.00020 0.90404 0.32258 0.30155

53 H(1) -0.00064 -2.87668 -1.02647 -0.95956

54 H(1) -0.00064 -2.87668 -1.02647 -0.95956

55 H(1) 0.00020 0.90404 0.32258 0.30155

56 H(1) 0.00020 0.90404 0.32258 0.30155

57 H(1) -0.00064 -2.87668 -1.02647 -0.95956

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

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

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1 Atom 0.008628 0.012872 -0.021500

2 Atom -0.035067 -0.036210 0.071277

3 Atom -0.094514 -0.094472 0.188987

4 Atom 0.006839 0.007726 -0.014565

5 Atom -0.027632 -0.027679 0.055312

6 Atom 0.062169 0.047477 -0.109646

7 Atom -0.094514 -0.094472 0.188987

8 Atom -0.035067 -0.036210 0.071277

9 Atom 0.008628 0.012872 -0.021500

10 Atom -0.027632 -0.027679 0.055312

11 Atom 0.006839 0.007726 -0.014565

12 Atom -0.188497 -0.189914 0.378411

13 Atom -0.027632 -0.027679 0.055312

14 Atom 0.006839 0.007726 -0.014565

15 Atom -0.094514 -0.094472 0.188987

16 Atom -0.035067 -0.036210 0.071277

17 Atom 0.008628 0.012872 -0.021500

18 Atom 0.062169 0.047477 -0.109646

19 Atom -0.035067 -0.036210 0.071277

20 Atom -0.094514 -0.094472 0.188987

21 Atom 0.006839 0.007726 -0.014565

22 Atom -0.027632 -0.027679 0.055312

23 Atom 0.008628 0.012872 -0.021500

24 Atom -0.188497 -0.189914 0.378411

25 Atom 0.005625 -0.006785 0.001159

26 Atom 0.011520 0.011296 -0.022817

27 Atom -0.022736 -0.024477 0.047213

28 Atom 0.009124 0.007838 -0.016961

29 Atom -0.017722 -0.016890 0.034612

30 Atom 0.011520 0.011296 -0.022817

31 Atom -0.022736 -0.024477 0.047213

32 Atom 0.009124 0.007838 -0.016961

33 Atom -0.017722 -0.016890 0.034612

34 Atom -0.017722 -0.016890 0.034612

35 Atom 0.009124 0.007838 -0.016961

36 Atom -0.022736 -0.024477 0.047213

37 Atom 0.011520 0.011296 -0.022817

38 Atom 0.011520 0.011296 -0.022817

39 Atom -0.022736 -0.024477 0.047213

40 Atom 0.009124 0.007838 -0.016961

41 Atom -0.017722 -0.016890 0.034612

42 Atom 0.001109 0.000407 -0.001516

43 Atom -0.000148 0.001344 -0.001197

44 Atom 0.001109 0.000407 -0.001516

45 Atom -0.000148 0.001344 -0.001197

46 Atom -0.000148 0.001344 -0.001197

47 Atom 0.001109 0.000407 -0.001516

48 Atom 0.001109 0.000407 -0.001516

49 Atom -0.000148 0.001344 -0.001197

50 Atom 0.000977 -0.000189 -0.000788

51 Atom 0.002901 -0.002401 -0.000499

52 Atom 0.000977 -0.000189 -0.000788

53 Atom 0.002901 -0.002401 -0.000499

54 Atom 0.002901 -0.002401 -0.000499

55 Atom 0.000977 -0.000189 -0.000788

56 Atom 0.000977 -0.000189 -0.000788

57 Atom 0.002901 -0.002401 -0.000499

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XY XZ YZ

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1 Atom -0.006963 -0.000739 -0.000460

2 Atom -0.001336 0.005906 0.007354

3 Atom 0.002494 0.003534 0.008144

4 Atom 0.002757 -0.000991 -0.000647

5 Atom 0.000572 0.002550 0.003008

6 Atom 0.000000 0.000000 -0.002847

7 Atom -0.002494 -0.003534 0.008144

8 Atom 0.001336 -0.005906 0.007354

9 Atom 0.006963 0.000739 -0.000460

10 Atom -0.000572 -0.002550 0.003008

11 Atom -0.002757 0.000991 -0.000647

12 Atom 0.000000 0.013574 0.000000

13 Atom -0.000572 0.002550 -0.003008

14 Atom -0.002757 -0.000991 0.000647

15 Atom -0.002494 0.003534 -0.008144

16 Atom 0.001336 0.005906 -0.007354

17 Atom 0.006963 -0.000739 0.000460

18 Atom 0.000000 0.000000 0.002847

19 Atom -0.001336 -0.005906 -0.007354

20 Atom 0.002494 -0.003534 -0.008144

21 Atom 0.002757 0.000991 0.000647

22 Atom 0.000572 -0.002550 -0.003008

23 Atom -0.006963 0.000739 0.000460

24 Atom 0.000000 -0.013574 0.000000

25 Atom 0.000000 0.000000 0.000000

26 Atom -0.002145 -0.000771 0.000705

27 Atom -0.001085 0.001380 -0.001229

28 Atom -0.000040 -0.000458 0.000500

29 Atom -0.000824 0.000947 -0.001040

30 Atom 0.002145 0.000771 0.000705

31 Atom 0.001085 -0.001380 -0.001229

32 Atom 0.000040 0.000458 0.000500

33 Atom 0.000824 -0.000947 -0.001040

34 Atom -0.000824 -0.000947 0.001040

35 Atom -0.000040 0.000458 -0.000500

36 Atom -0.001085 -0.001380 0.001229

37 Atom -0.002145 0.000771 -0.000705

38 Atom 0.002145 -0.000771 -0.000705

39 Atom 0.001085 0.001380 0.001229

40 Atom 0.000040 -0.000458 -0.000500

41 Atom 0.000824 0.000947 0.001040

42 Atom -0.002110 -0.000082 0.000073

43 Atom 0.001566 0.000030 0.000032

44 Atom 0.002110 0.000082 0.000073

45 Atom -0.001566 -0.000030 0.000032

46 Atom 0.001566 -0.000030 -0.000032

47 Atom -0.002110 0.000082 -0.000073

48 Atom 0.002110 -0.000082 -0.000073

49 Atom -0.001566 0.000030 -0.000032

50 Atom -0.000199 0.000036 -0.000011

51 Atom -0.002224 0.000111 -0.000012

52 Atom 0.000199 -0.000036 -0.000011

53 Atom 0.002224 -0.000111 -0.000012

54 Atom -0.002224 -0.000111 0.000012

55 Atom -0.000199 -0.000036 0.000011

56 Atom 0.000199 0.000036 0.000011

57 Atom 0.002224 0.000111 0.000012

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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 -0.0215 -2.889 -1.031 -0.964 0.0289 0.0192 0.9994

1 C(13) Bbb 0.0035 0.470 0.168 0.157 0.8030 0.5950 -0.0347

Bcc 0.0180 2.419 0.863 0.807 -0.5953 0.8035 0.0018

Baa -0.0379 -1.462 -0.522 -0.488 0.5655 0.8202 -0.0858

2 N(14) Bbb -0.0342 -1.319 -0.471 -0.440 0.8229 -0.5681 -0.0065

Bcc 0.0721 2.780 0.992 0.927 0.0541 0.0670 0.9963

Baa -0.0970 -13.020 -4.646 -4.343 -0.6962 0.7178 -0.0118

3 C(13) Bbb -0.0922 -12.378 -4.417 -4.129 0.7178 0.6957 -0.0292

Bcc 0.1893 25.398 9.063 8.472 0.0127 0.0288 0.9995

Baa -0.0146 -1.962 -0.700 -0.655 0.0431 0.0236 0.9988

4 C(13) Bbb 0.0045 0.603 0.215 0.201 0.7588 -0.6511 -0.0173

Bcc 0.0101 1.359 0.485 0.453 0.6499 0.7587 -0.0459

Baa -0.0282 -3.788 -1.352 -1.264 -0.6780 0.7350 -0.0058

5 C(13) Bbb -0.0273 -3.659 -1.306 -1.221 0.7344 0.6771 -0.0473

Bcc 0.0555 7.448 2.657 2.484 0.0309 0.0363 0.9989

Baa -0.1097 -4.231 -1.510 -1.411 0.0000 0.0181 0.9998

6 N(14) Bbb 0.0475 1.833 0.654 0.611 0.0000 0.9998 -0.0181

Bcc 0.0622 2.398 0.856 0.800 1.0000 0.0000 0.0000

Baa -0.0970 -13.020 -4.646 -4.343 0.6962 0.7178 -0.0118

7 C(13) Bbb -0.0922 -12.378 -4.417 -4.129 0.7178 -0.6957 0.0292

Bcc 0.1893 25.398 9.063 8.472 -0.0127 0.0288 0.9995

Baa -0.0379 -1.462 -0.522 -0.488 -0.5655 0.8202 -0.0858

8 N(14) Bbb -0.0342 -1.319 -0.471 -0.440 0.8229 0.5681 0.0065

Bcc 0.0721 2.780 0.992 0.927 -0.0541 0.0670 0.9963

Baa -0.0215 -2.889 -1.031 -0.964 -0.0289 0.0192 0.9994

9 C(13) Bbb 0.0035 0.470 0.168 0.157 0.8030 -0.5950 0.0347

Bcc 0.0180 2.419 0.863 0.807 0.5953 0.8035 0.0018

Baa -0.0282 -3.788 -1.352 -1.264 0.6780 0.7350 -0.0058

10 C(13) Bbb -0.0273 -3.659 -1.306 -1.221 0.7344 -0.6771 0.0473

Bcc 0.0555 7.448 2.657 2.484 -0.0309 0.0363 0.9989

Baa -0.0146 -1.962 -0.700 -0.655 -0.0431 0.0236 0.9988

11 C(13) Bbb 0.0045 0.603 0.215 0.201 0.7588 0.6511 0.0173

Bcc 0.0101 1.359 0.485 0.453 -0.6499 0.7587 -0.0459

Baa -0.1899 -7.325 -2.614 -2.443 0.0000 1.0000 0.0000

12 N(14) Bbb -0.1888 -7.282 -2.599 -2.429 0.9997 0.0000 -0.0239

Bcc 0.3787 14.607 5.212 4.872 0.0239 0.0000 0.9997

Baa -0.0282 -3.788 -1.352 -1.264 0.6780 0.7350 0.0058

13 C(13) Bbb -0.0273 -3.659 -1.306 -1.221 0.7344 -0.6771 -0.0473

Bcc 0.0555 7.448 2.657 2.484 0.0309 -0.0363 0.9989

Baa -0.0146 -1.962 -0.700 -0.655 0.0431 -0.0236 0.9988

14 C(13) Bbb 0.0045 0.603 0.215 0.201 0.7588 0.6511 -0.0173

Bcc 0.0101 1.359 0.485 0.453 -0.6499 0.7587 0.0459

Baa -0.0970 -13.020 -4.646 -4.343 0.6962 0.7178 0.0118

15 C(13) Bbb -0.0922 -12.378 -4.417 -4.129 0.7178 -0.6957 -0.0292

Bcc 0.1893 25.398 9.063 8.472 0.0127 -0.0288 0.9995

Baa -0.0379 -1.462 -0.522 -0.488 -0.5655 0.8202 0.0858

16 N(14) Bbb -0.0342 -1.319 -0.471 -0.440 0.8229 0.5681 -0.0065

Bcc 0.0721 2.780 0.992 0.927 0.0541 -0.0670 0.9963

Baa -0.0215 -2.889 -1.031 -0.964 0.0289 -0.0192 0.9994

17 C(13) Bbb 0.0035 0.470 0.168 0.157 0.8030 -0.5950 -0.0347

Bcc 0.0180 2.419 0.863 0.807 0.5953 0.8035 -0.0018

Baa -0.1097 -4.231 -1.510 -1.411 0.0000 -0.0181 0.9998

18 N(14) Bbb 0.0475 1.833 0.654 0.611 0.0000 0.9998 0.0181

Bcc 0.0622 2.398 0.856 0.800 1.0000 0.0000 0.0000

Baa -0.0379 -1.462 -0.522 -0.488 0.5655 0.8202 0.0858

19 N(14) Bbb -0.0342 -1.319 -0.471 -0.440 0.8229 -0.5681 0.0065

Bcc 0.0721 2.780 0.992 0.927 -0.0541 -0.0670 0.9963

Baa -0.0970 -13.020 -4.646 -4.343 -0.6962 0.7178 0.0118

20 C(13) Bbb -0.0922 -12.378 -4.417 -4.129 0.7178 0.6957 0.0292

Bcc 0.1893 25.398 9.063 8.472 -0.0127 -0.0288 0.9995

Baa -0.0146 -1.962 -0.700 -0.655 -0.0431 -0.0236 0.9988

21 C(13) Bbb 0.0045 0.603 0.215 0.201 0.7588 -0.6511 0.0173

Bcc 0.0101 1.359 0.485 0.453 0.6499 0.7587 0.0459

Baa -0.0282 -3.788 -1.352 -1.264 -0.6780 0.7350 0.0058

22 C(13) Bbb -0.0273 -3.659 -1.306 -1.221 0.7344 0.6771 0.0473

Bcc 0.0555 7.448 2.657 2.484 -0.0309 -0.0363 0.9989

Baa -0.0215 -2.889 -1.031 -0.964 -0.0289 -0.0192 0.9994

23 C(13) Bbb 0.0035 0.470 0.168 0.157 0.8030 0.5950 0.0347

Bcc 0.0180 2.419 0.863 0.807 -0.5953 0.8035 -0.0018

Baa -0.1899 -7.325 -2.614 -2.443 0.0000 1.0000 0.0000

24 N(14) Bbb -0.1888 -7.282 -2.599 -2.429 0.9997 0.0000 0.0239

Bcc 0.3787 14.607 5.212 4.872 -0.0239 0.0000 0.9997

Baa -0.0068 -0.227 -0.081 -0.076 0.0000 1.0000 0.0000

25 Zn(67) Bbb 0.0012 0.039 0.014 0.013 0.0000 0.0000 1.0000

Bcc 0.0056 0.188 0.067 0.063 1.0000 0.0000 0.0000

Baa -0.0228 -3.066 -1.094 -1.023 0.0212 -0.0193 0.9996

26 C(13) Bbb 0.0093 1.243 0.443 0.414 0.6883 0.7254 -0.0006

Bcc 0.0136 1.823 0.651 0.608 0.7251 -0.6881 -0.0287

Baa -0.0250 -3.355 -1.197 -1.119 0.4285 0.9035 0.0072

27 C(13) Bbb -0.0223 -2.987 -1.066 -0.996 0.9033 -0.4282 -0.0255

Bcc 0.0473 6.342 2.263 2.116 0.0200 -0.0174 0.9996

Baa -0.0170 -2.278 -0.813 -0.760 0.0175 -0.0201 0.9996

28 C(13) Bbb 0.0078 1.053 0.376 0.351 0.0385 0.9991 0.0194

Bcc 0.0091 1.226 0.437 0.409 0.9991 -0.0381 -0.0183

Baa -0.0182 -2.446 -0.873 -0.816 0.8535 0.5210 -0.0050

29 C(13) Bbb -0.0164 -2.203 -0.786 -0.735 -0.5207 0.8533 0.0271

Bcc 0.0347 4.650 1.659 1.551 0.0184 -0.0205 0.9996

Baa -0.0228 -3.066 -1.094 -1.023 -0.0212 -0.0193 0.9996

30 C(13) Bbb 0.0093 1.243 0.443 0.414 -0.6883 0.7254 -0.0006

Bcc 0.0136 1.823 0.651 0.608 0.7251 0.6881 0.0287

Baa -0.0250 -3.355 -1.197 -1.119 -0.4285 0.9035 0.0072

31 C(13) Bbb -0.0223 -2.987 -1.066 -0.996 0.9033 0.4282 0.0255

Bcc 0.0473 6.342 2.263 2.116 -0.0200 -0.0174 0.9996

Baa -0.0170 -2.278 -0.813 -0.760 -0.0175 -0.0201 0.9996

32 C(13) Bbb 0.0078 1.053 0.376 0.351 -0.0385 0.9991 0.0194

Bcc 0.0091 1.226 0.437 0.409 0.9991 0.0381 0.0183

Baa -0.0182 -2.446 -0.873 -0.816 0.8535 -0.5210 0.0050

33 C(13) Bbb -0.0164 -2.203 -0.786 -0.735 0.5207 0.8533 0.0271

Bcc 0.0347 4.650 1.659 1.551 -0.0184 -0.0205 0.9996

Baa -0.0182 -2.446 -0.873 -0.816 0.8535 0.5210 0.0050

34 C(13) Bbb -0.0164 -2.203 -0.786 -0.735 -0.5207 0.8533 -0.0271

Bcc 0.0347 4.650 1.659 1.551 -0.0184 0.0205 0.9996

Baa -0.0170 -2.278 -0.813 -0.760 -0.0175 0.0201 0.9996

35 C(13) Bbb 0.0078 1.053 0.376 0.351 0.0385 0.9991 -0.0194

Bcc 0.0091 1.226 0.437 0.409 0.9991 -0.0381 0.0183

Baa -0.0250 -3.355 -1.197 -1.119 0.4285 0.9035 -0.0072

36 C(13) Bbb -0.0223 -2.987 -1.066 -0.996 0.9033 -0.4282 0.0255

Bcc 0.0473 6.342 2.263 2.116 -0.0200 0.0174 0.9996

Baa -0.0228 -3.066 -1.094 -1.023 -0.0212 0.0193 0.9996

37 C(13) Bbb 0.0093 1.243 0.443 0.414 0.6883 0.7254 0.0006

Bcc 0.0136 1.823 0.651 0.608 0.7251 -0.6881 0.0287

Baa -0.0228 -3.066 -1.094 -1.023 0.0212 0.0193 0.9996

38 C(13) Bbb 0.0093 1.243 0.443 0.414 -0.6883 0.7254 0.0006

Bcc 0.0136 1.823 0.651 0.608 0.7251 0.6881 -0.0287

Baa -0.0250 -3.355 -1.197 -1.119 -0.4285 0.9035 -0.0072

39 C(13) Bbb -0.0223 -2.987 -1.066 -0.996 0.9033 0.4282 -0.0255

Bcc 0.0473 6.342 2.263 2.116 0.0200 0.0174 0.9996

Baa -0.0170 -2.278 -0.813 -0.760 0.0175 0.0201 0.9996

40 C(13) Bbb 0.0078 1.053 0.376 0.351 -0.0385 0.9991 -0.0194

Bcc 0.0091 1.226 0.437 0.409 0.9991 0.0381 -0.0183

Baa -0.0182 -2.446 -0.873 -0.816 0.8535 -0.5210 -0.0050

41 C(13) Bbb -0.0164 -2.203 -0.786 -0.735 0.5207 0.8533 -0.0271

Bcc 0.0347 4.650 1.659 1.551 0.0184 0.0205 0.9996

Baa -0.0015 -0.810 -0.289 -0.270 0.0046 -0.0330 0.9994

42 H(1) Bbb -0.0014 -0.737 -0.263 -0.246 0.6467 0.7624 0.0222

Bcc 0.0029 1.547 0.552 0.516 0.7627 -0.6462 -0.0249

Baa -0.0012 -0.639 -0.228 -0.213 -0.1170 0.0596 0.9913

43 H(1) Bbb -0.0011 -0.606 -0.216 -0.202 0.8375 -0.5306 0.1308

Bcc 0.0023 1.245 0.444 0.415 0.5338 0.8455 0.0122

Baa -0.0015 -0.810 -0.289 -0.270 -0.0046 -0.0330 0.9994

44 H(1) Bbb -0.0014 -0.737 -0.263 -0.246 -0.6467 0.7624 0.0222

Bcc 0.0029 1.547 0.552 0.516 0.7627 0.6462 0.0249

Baa -0.0012 -0.639 -0.228 -0.213 0.1170 0.0596 0.9913

45 H(1) Bbb -0.0011 -0.606 -0.216 -0.202 0.8375 0.5306 -0.1308

Bcc 0.0023 1.245 0.444 0.415 -0.5338 0.8455 0.0122

Baa -0.0012 -0.639 -0.228 -0.213 0.1170 -0.0596 0.9913

46 H(1) Bbb -0.0011 -0.606 -0.216 -0.202 0.8375 -0.5306 -0.1308

Bcc 0.0023 1.245 0.444 0.415 0.5338 0.8455 -0.0122

Baa -0.0015 -0.810 -0.289 -0.270 -0.0046 0.0330 0.9994

47 H(1) Bbb -0.0014 -0.737 -0.263 -0.246 0.6467 0.7624 -0.0222

Bcc 0.0029 1.547 0.552 0.516 0.7627 -0.6462 0.0249

Baa -0.0015 -0.810 -0.289 -0.270 0.0046 0.0330 0.9994

48 H(1) Bbb -0.0014 -0.737 -0.263 -0.246 -0.6467 0.7624 -0.0222

Bcc 0.0029 1.547 0.552 0.516 0.7627 0.6462 -0.0249

Baa -0.0012 -0.639 -0.228 -0.213 -0.1170 -0.0596 0.9913

49 H(1) Bbb -0.0011 -0.606 -0.216 -0.202 0.8375 0.5306 0.1308

Bcc 0.0023 1.245 0.444 0.415 -0.5338 0.8455 -0.0122

Baa -0.0008 -0.421 -0.150 -0.140 -0.0188 0.0126 0.9997

50 H(1) Bbb -0.0002 -0.119 -0.042 -0.040 0.1636 0.9865 -0.0094

Bcc 0.0010 0.539 0.192 0.180 0.9863 -0.1634 0.0206

Baa -0.0032 -1.713 -0.611 -0.572 0.3421 0.9396 -0.0098

51 H(1) Bbb -0.0005 -0.268 -0.096 -0.089 -0.0208 0.0180 0.9996

Bcc 0.0037 1.981 0.707 0.661 0.9394 -0.3418 0.0257

Baa -0.0008 -0.421 -0.150 -0.140 0.0188 0.0126 0.9997

52 H(1) Bbb -0.0002 -0.119 -0.042 -0.040 -0.1636 0.9865 -0.0094

Bcc 0.0010 0.539 0.192 0.180 0.9863 0.1634 -0.0206

Baa -0.0032 -1.713 -0.611 -0.572 -0.3421 0.9396 -0.0098

53 H(1) Bbb -0.0005 -0.268 -0.096 -0.089 0.0208 0.0180 0.9996

Bcc 0.0037 1.981 0.707 0.661 0.9394 0.3418 -0.0257

Baa -0.0032 -1.713 -0.611 -0.572 0.3421 0.9396 0.0098

54 H(1) Bbb -0.0005 -0.268 -0.096 -0.089 0.0208 -0.0180 0.9996

Bcc 0.0037 1.981 0.707 0.661 0.9394 -0.3418 -0.0257

Baa -0.0008 -0.421 -0.150 -0.140 0.0188 -0.0126 0.9997

55 H(1) Bbb -0.0002 -0.119 -0.042 -0.040 0.1636 0.9865 0.0094

Bcc 0.0010 0.539 0.192 0.180 0.9863 -0.1634 -0.0206

Baa -0.0008 -0.421 -0.150 -0.140 -0.0188 -0.0126 0.9997

56 H(1) Bbb -0.0002 -0.119 -0.042 -0.040 -0.1636 0.9865 0.0094

Bcc 0.0010 0.539 0.192 0.180 0.9863 0.1634 0.0206

Baa -0.0032 -1.713 -0.611 -0.572 -0.3421 0.9396 0.0098

57 H(1) Bbb -0.0005 -0.268 -0.096 -0.089 -0.0208 -0.0180 0.9996

Bcc 0.0037 1.981 0.707 0.661 0.9394 0.3418 0.0257

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

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Sat Jun 15 12:08:46 2019, MaxMem= 1342177280 cpu: 50.3

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

Compute integral first derivatives.

... and contract with generalized density number 0.

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

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 32896 NPrTT= 163506 LenC2= 22819 LenP2D= 61244.

LDataN: DoStor=T MaxTD1= 6 Len= 172

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

GePol: Maximum number of non-zero 1st derivatives = 199

Leave Link 701 at Sat Jun 15 12:08:55 2019, MaxMem= 1342177280 cpu: 103.7

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

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

Leave Link 702 at Sat Jun 15 12:08:56 2019, MaxMem= 1342177280 cpu: 3.5

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

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=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= 800

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Sat Jun 15 12:09:16 2019, MaxMem= 1342177280 cpu: 228.4

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

Dipole = 9.94759830D-14 5.86197757D-14 8.59163674D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000732653 -0.002885362 -0.000215846

2 7 0.003259801 0.002327264 0.000353437

3 6 -0.002835104 0.000295573 -0.000269478

4 6 0.000898563 0.000140601 -0.000006199

5 6 0.000346196 0.001110114 -0.000038030

6 7 0.000000000 -0.002048515 0.000145739

7 6 0.002835104 0.000295573 -0.000269478

8 7 -0.003259801 0.002327264 0.000353437

9 6 0.000732653 -0.002885362 -0.000215846

10 6 -0.000346196 0.001110114 -0.000038030

11 6 -0.000898563 0.000140601 -0.000006199

12 7 -0.002122903 0.000000000 0.000126010

13 6 0.000346196 -0.001110114 -0.000038030

14 6 0.000898563 -0.000140601 -0.000006199

15 6 -0.002835104 -0.000295573 -0.000269478

16 7 0.003259801 -0.002327264 0.000353437

17 6 -0.000732653 0.002885362 -0.000215846

18 7 0.000000000 0.002048515 0.000145739

19 7 -0.003259801 -0.002327264 0.000353437

20 6 0.002835104 -0.000295573 -0.000269478

21 6 -0.000898563 -0.000140601 -0.000006199

22 6 -0.000346196 -0.001110114 -0.000038030

23 6 0.000732653 0.002885362 -0.000215846

24 7 0.002122903 0.000000000 0.000126010

25 30 0.000000000 0.000000000 -0.000414524

26 6 -0.001563186 -0.002683409 -0.000050872

27 6 -0.002614276 0.001317930 0.000086257

28 6 -0.001386188 0.002621208 0.000081426

29 6 0.002715168 0.001522812 -0.000033604

30 6 0.001563186 -0.002683409 -0.000050872

31 6 0.002614276 0.001317930 0.000086257

32 6 0.001386188 0.002621208 0.000081426

33 6 -0.002715168 0.001522812 -0.000033604

34 6 -0.002715168 -0.001522812 -0.000033604

35 6 0.001386188 -0.002621208 0.000081426

36 6 0.002614276 -0.001317930 0.000086257

37 6 0.001563186 0.002683409 -0.000050872

38 6 -0.001563186 0.002683409 -0.000050872

39 6 -0.002614276 -0.001317930 0.000086257

40 6 -0.001386188 -0.002621208 0.000081426

41 6 0.002715168 -0.001522812 -0.000033604

42 1 -0.000757864 -0.000561397 0.000011928

43 1 0.000562505 0.000732660 0.000007331

44 1 0.000757864 -0.000561397 0.000011928

45 1 -0.000562505 0.000732660 0.000007331

46 1 -0.000562505 -0.000732660 0.000007331

47 1 0.000757864 0.000561397 0.000011928

48 1 -0.000757864 0.000561397 0.000011928

49 1 0.000562505 -0.000732660 0.000007331

50 1 0.000248291 -0.000929702 0.000020473

51 1 0.000936160 -0.000247015 0.000020932

52 1 -0.000248291 -0.000929702 0.000020473

53 1 -0.000936160 -0.000247015 0.000020932

54 1 -0.000936160 0.000247015 0.000020932

55 1 -0.000248291 0.000929702 0.000020473

56 1 0.000248291 0.000929702 0.000020473

57 1 0.000936160 0.000247015 0.000020932

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

Cartesian Forces: Max 0.003259801 RMS 0.001369610

Leave Link 716 at Sat Jun 15 12:09:19 2019, MaxMem= 1342177280 cpu: 8.0

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

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

Internal Forces: Max 0.004195477 RMS 0.001174592

Search for a local minimum.

Step number 1 out of a maximum of 342

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

RMS Force = .11746D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Second derivative matrix not updated -- first step.

ITU= 0

Eigenvalues --- 0.01571 0.01587 0.01610 0.01614 0.01624

Eigenvalues --- 0.01645 0.01681 0.01697 0.01763 0.01768

Eigenvalues --- 0.01776 0.01780 0.01781 0.01783 0.01783

Eigenvalues --- 0.01794 0.01835 0.01846 0.01891 0.01894

Eigenvalues --- 0.01903 0.01957 0.01958 0.02008 0.02008

Eigenvalues --- 0.02008 0.02008 0.02051 0.02051 0.02051

Eigenvalues --- 0.02051 0.02053 0.02053 0.02053 0.02053

Eigenvalues --- 0.02077 0.02113 0.02113 0.02113 0.02113

Eigenvalues --- 0.02119 0.02119 0.02119 0.02119 0.02124

Eigenvalues --- 0.02124 0.02124 0.02124 0.02245 0.02249

Eigenvalues --- 0.02324 0.02335 0.03347 0.03901 0.03919

Eigenvalues --- 0.07464 0.15215 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 0.16000 0.16238 0.16348

Eigenvalues --- 0.17211 0.22000 0.22000 0.22000 0.22000

Eigenvalues --- 0.22599 0.22600 0.22600 0.22606 0.24075

Eigenvalues --- 0.24274 0.24508 0.24509 0.24521 0.24530

Eigenvalues --- 0.24597 0.24605 0.24825 0.24946 0.24947

Eigenvalues --- 0.24955 0.24984 0.24998 0.24998 0.24998

Eigenvalues --- 0.24998 0.33739 0.34078 0.34263 0.34315

Eigenvalues --- 0.34822 0.34872 0.35074 0.35218 0.35218

Eigenvalues --- 0.35218 0.35218 0.35231 0.35243 0.35243

Eigenvalues --- 0.35243 0.35243 0.35247 0.35247 0.35247

Eigenvalues --- 0.35247 0.35252 0.35252 0.35252 0.35252

Eigenvalues --- 0.37368 0.37390 0.37553 0.37567 0.40819

Eigenvalues --- 0.40903 0.41950 0.41951 0.41966 0.41979

Eigenvalues --- 0.41986 0.42301 0.43209 0.43248 0.44583

Eigenvalues --- 0.45129 0.45211 0.45217 0.45344 0.45791

Eigenvalues --- 0.45910 0.45911 0.45919 0.45942 0.46127

Eigenvalues --- 0.46178 0.46180 0.46180 0.46184 0.46684

Eigenvalues --- 0.48980 0.50406 0.50867 0.51351 0.53511

Eigenvalues --- 0.55376 0.55383 0.55601 0.58016 0.58041

RFO step: Lambda=-1.23532379D-03 EMin= 1.57050720D-02

Linear search not attempted -- first point.

Iteration 1 RMS(Cart)= 0.01102000 RMS(Int)= 0.00000829

Iteration 2 RMS(Cart)= 0.00002053 RMS(Int)= 0.00000215

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000215

ITry= 1 IFail=0 DXMaxC= 3.03D-02 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.23D-11 for atom 54.

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

(Linear) (Quad) (Total)

R1 2.56770 -0.00295 0.00000 -0.00542 -0.00542 2.56228

R2 2.76896 -0.00182 0.00000 -0.00526 -0.00526 2.76370

R3 2.54413 -0.00308 0.00000 -0.00677 -0.00677 2.53736

R4 2.62321 -0.00202 0.00000 -0.00406 -0.00406 2.61915

R5 3.88762 -0.00180 0.00000 -0.00549 -0.00549 3.88213

R6 2.75105 -0.00212 0.00000 -0.00578 -0.00578 2.74527

R7 2.51963 -0.00317 0.00000 -0.00660 -0.00661 2.51302

R8 2.68625 -0.00236 0.00000 -0.00602 -0.00602 2.68023

R9 2.64754 -0.00346 0.00000 -0.00750 -0.00750 2.64004

R10 2.64185 -0.00354 0.00000 -0.00761 -0.00761 2.63424

R11 2.51963 -0.00317 0.00000 -0.00660 -0.00661 2.51302

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R13 2.75105 -0.00212 0.00000 -0.00578 -0.00578 2.74527

R14 2.56770 -0.00295 0.00000 -0.00542 -0.00542 2.56228

R15 3.88762 -0.00180 0.00000 -0.00549 -0.00549 3.88213

R16 2.76896 -0.00182 0.00000 -0.00526 -0.00526 2.76370

R17 2.54413 -0.00308 0.00000 -0.00677 -0.00677 2.53736

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D4 0.19057 0.00003 0.00000 -0.00303 -0.00303 0.18755

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D96 -3.13853 0.00001 0.00000 0.00046 0.00046 -3.13807

D97 3.13942 -0.00003 0.00000 -0.00136 -0.00136 3.13806

D98 -0.00360 -0.00002 0.00000 -0.00119 -0.00119 -0.00479

D99 0.00530 0.00005 0.00000 0.00287 0.00287 0.00818

D100 -2.96331 0.00002 0.00000 -0.00323 -0.00324 -2.96654

D101 -3.12082 0.00007 0.00000 0.00336 0.00337 -3.11745

D102 0.19375 0.00004 0.00000 -0.00274 -0.00274 0.19101

D103 -3.11565 0.00012 0.00000 0.00256 0.00256 -3.11309

D104 0.00804 0.00008 0.00000 0.00198 0.00198 0.01002

D105 3.12606 -0.00007 0.00000 -0.00321 -0.00322 3.12284

D106 -0.00496 -0.00004 0.00000 -0.00265 -0.00266 -0.00762

D107 -0.19057 -0.00003 0.00000 0.00303 0.00303 -0.18755

D108 2.96160 0.00000 0.00000 0.00359 0.00359 2.96518

D109 -3.06665 0.00033 0.00000 0.00452 0.00452 -3.06213

D110 -1.66823 0.00013 0.00000 0.00359 0.00359 -1.66464

D111 -0.27356 -0.00006 0.00000 0.00271 0.00270 -0.27085

D112 0.27311 0.00005 0.00000 -0.00296 -0.00296 0.27015

D113 1.67153 -0.00014 0.00000 -0.00389 -0.00388 1.66765

D114 3.06620 -0.00033 0.00000 -0.00477 -0.00477 3.06143

D115 -0.00804 -0.00008 0.00000 -0.00198 -0.00198 -0.01002

D116 3.11565 -0.00012 0.00000 -0.00256 -0.00256 3.11309

D117 3.12082 -0.00007 0.00000 -0.00336 -0.00337 3.11745

D118 -0.00530 -0.00005 0.00000 -0.00287 -0.00287 -0.00818

D119 -0.19375 -0.00004 0.00000 0.00274 0.00274 -0.19101

D120 2.96331 -0.00002 0.00000 0.00323 0.00324 2.96654

D121 0.00496 0.00004 0.00000 0.00265 0.00266 0.00762

D122 -3.12606 0.00007 0.00000 0.00321 0.00322 -3.12284

D123 -2.96160 0.00000 0.00000 -0.00359 -0.00359 -2.96518

D124 0.19057 0.00003 0.00000 -0.00303 -0.00303 0.18755

D125 1.66823 -0.00013 0.00000 -0.00359 -0.00359 1.66464

D126 3.06665 -0.00033 0.00000 -0.00452 -0.00452 3.06213

D127 0.27356 0.00006 0.00000 -0.00271 -0.00270 0.27085

D128 -1.67153 0.00014 0.00000 0.00389 0.00388 -1.66765

D129 -0.27311 -0.00005 0.00000 0.00296 0.00296 -0.27015

D130 -3.06620 0.00033 0.00000 0.00477 0.00477 -3.06143

D131 -3.12310 0.00004 0.00000 0.00233 0.00233 -3.12077

D132 0.01249 0.00001 0.00000 0.00085 0.00085 0.01334

D133 0.00347 0.00003 0.00000 0.00190 0.00190 0.00538

D134 3.13907 0.00000 0.00000 0.00042 0.00042 3.13949

D135 -0.00054 -0.00001 0.00000 -0.00034 -0.00034 -0.00088

D136 3.13783 -0.00003 0.00000 -0.00131 -0.00131 3.13652

D137 -3.13705 0.00002 0.00000 0.00092 0.00092 -3.13613

D138 0.00132 0.00000 0.00000 -0.00005 -0.00005 0.00128

D139 -3.13942 0.00003 0.00000 0.00136 0.00136 -3.13806

D140 0.00360 0.00002 0.00000 0.00119 0.00119 0.00479

D141 -0.00450 0.00000 0.00000 -0.00028 -0.00028 -0.00478

D142 3.13853 -0.00001 0.00000 -0.00046 -0.00046 3.13807

D143 -0.00264 -0.00002 0.00000 -0.00138 -0.00138 -0.00402

D144 3.12895 -0.00004 0.00000 -0.00187 -0.00187 3.12709

D145 -3.14049 0.00001 0.00000 -0.00025 -0.00025 -3.14074

D146 -0.00890 -0.00002 0.00000 -0.00075 -0.00074 -0.00964

D147 0.00273 0.00001 0.00000 0.00038 0.00038 0.00311

D148 -3.13966 0.00001 0.00000 0.00029 0.00029 -3.13937

D149 3.14014 -0.00002 0.00000 -0.00088 -0.00087 3.13926

D150 -0.00225 -0.00002 0.00000 -0.00096 -0.00096 -0.00321

D151 0.01758 0.00008 0.00000 0.00200 0.00200 0.01957

D152 -3.11198 0.00012 0.00000 0.00264 0.00264 -3.10934

D153 0.00356 0.00001 0.00000 0.00038 0.00038 0.00393

D154 -3.13885 0.00000 0.00000 0.00002 0.00002 -3.13883

D155 -3.13883 0.00001 0.00000 0.00029 0.00029 -3.13854

D156 0.00195 0.00000 0.00000 -0.00007 -0.00007 0.00188

D157 -0.00035 0.00000 0.00000 -0.00005 -0.00005 -0.00039

D158 3.14086 -0.00001 0.00000 -0.00039 -0.00039 3.14047

D159 -3.14113 0.00001 0.00000 0.00031 0.00031 -3.14082

D160 0.00007 0.00000 0.00000 -0.00003 -0.00003 0.00004

D161 -0.00370 -0.00001 0.00000 -0.00029 -0.00029 -0.00399

D162 3.13932 -0.00001 0.00000 -0.00046 -0.00046 3.13886

D163 3.13828 0.00000 0.00000 0.00006 0.00006 3.13834

D164 -0.00188 0.00000 0.00000 -0.00011 -0.00011 -0.00199

D165 -0.00356 -0.00001 0.00000 -0.00038 -0.00038 -0.00393

D166 3.13885 0.00000 0.00000 -0.00002 -0.00002 3.13883

D167 3.13883 -0.00001 0.00000 -0.00029 -0.00029 3.13854

D168 -0.00195 0.00000 0.00000 0.00007 0.00007 -0.00188

D169 0.00035 0.00000 0.00000 0.00005 0.00005 0.00039

D170 -3.14086 0.00001 0.00000 0.00039 0.00039 -3.14047

D171 3.14113 -0.00001 0.00000 -0.00031 -0.00031 3.14082

D172 -0.00007 0.00000 0.00000 0.00003 0.00003 -0.00004

D173 0.00370 0.00001 0.00000 0.00029 0.00029 0.00399

D174 -3.13932 0.00001 0.00000 0.00046 0.00046 -3.13886

D175 -3.13828 0.00000 0.00000 -0.00006 -0.00006 -3.13834

D176 0.00188 0.00000 0.00000 0.00011 0.00011 0.00199

D177 -0.00370 -0.00001 0.00000 -0.00029 -0.00029 -0.00399

D178 3.13828 0.00000 0.00000 0.00006 0.00006 3.13834

D179 3.13932 -0.00001 0.00000 -0.00046 -0.00046 3.13886

D180 -0.00188 0.00000 0.00000 -0.00011 -0.00011 -0.00199

D181 -0.00035 0.00000 0.00000 -0.00005 -0.00005 -0.00039

D182 -3.14113 0.00001 0.00000 0.00031 0.00031 -3.14082

D183 3.14086 -0.00001 0.00000 -0.00039 -0.00039 3.14047

D184 0.00007 0.00000 0.00000 -0.00003 -0.00003 0.00004

D185 0.00356 0.00001 0.00000 0.00038 0.00038 0.00393

D186 -3.13883 0.00001 0.00000 0.00029 0.00029 -3.13854

D187 -3.13885 0.00000 0.00000 0.00002 0.00002 -3.13883

D188 0.00195 0.00000 0.00000 -0.00007 -0.00007 0.00188

D189 -0.00356 -0.00001 0.00000 -0.00038 -0.00038 -0.00393

D190 3.13885 0.00000 0.00000 -0.00002 -0.00002 3.13883

D191 3.13883 -0.00001 0.00000 -0.00029 -0.00029 3.13854

D192 -0.00195 0.00000 0.00000 0.00007 0.00007 -0.00188

D193 0.00035 0.00000 0.00000 0.00005 0.00005 0.00039

D194 -3.14086 0.00001 0.00000 0.00039 0.00039 -3.14047

D195 3.14113 -0.00001 0.00000 -0.00031 -0.00031 3.14082

D196 -0.00007 0.00000 0.00000 0.00003 0.00003 -0.00004

D197 0.00370 0.00001 0.00000 0.00029 0.00029 0.00399

D198 -3.13932 0.00001 0.00000 0.00046 0.00046 -3.13886

D199 -3.13828 0.00000 0.00000 -0.00006 -0.00006 -3.13834

D200 0.00188 0.00000 0.00000 0.00011 0.00011 0.00199

Item Value Threshold Converged?

Maximum Force 0.004195 0.000450 NO

RMS Force 0.001175 0.000300 NO

Maximum Displacement 0.030277 0.001800 NO

RMS Displacement 0.011030 0.001200 NO

Predicted change in Energy=-6.199131D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jun 15 12:09:19 2019, MaxMem= 1342177280 cpu: 4.9

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

Stoichiometry C32H16N8Zn(1-,2)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C32H16N4)]

Deg. of freedom 43

Full point group C2V NOp 4

RotChk: IX=0 Diff= 1.95D-16

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 2.771922 1.184079 0.006670

2 7 0 1.437416 1.421962 0.037829

3 6 0 1.186139 2.784646 0.007179

4 6 0 2.464118 3.474046 -0.036761

5 6 0 3.466305 2.470434 -0.038033

6 7 0 0.000000 3.385862 -0.001472

7 6 0 -1.186139 2.784646 0.007179

8 7 0 -1.437416 1.421962 0.037829

9 6 0 -2.771922 1.184079 0.006670

10 6 0 -3.466305 2.470434 -0.038033

11 6 0 -2.464118 3.474046 -0.036761

12 7 0 3.405016 0.000000 0.001776

13 6 0 3.466305 -2.470434 -0.038033

14 6 0 2.464118 -3.474046 -0.036761

15 6 0 1.186139 -2.784646 0.007179

16 7 0 1.437416 -1.421962 0.037829

17 6 0 2.771922 -1.184079 0.006670

18 7 0 0.000000 -3.385862 -0.001472

19 7 0 -1.437416 -1.421962 0.037829

20 6 0 -1.186139 -2.784646 0.007179

21 6 0 -2.464118 -3.474046 -0.036761

22 6 0 -3.466305 -2.470434 -0.038033

23 6 0 -2.771922 -1.184079 0.006670

24 7 0 -3.405016 0.000000 0.001776

25 30 0 0.000000 0.000000 0.401365

26 6 0 4.818197 -2.807511 -0.082151

27 6 0 5.160857 -4.155937 -0.121197

28 6 0 4.167592 -5.152964 -0.120998

29 6 0 2.816546 -4.825170 -0.081479

30 6 0 -4.818197 -2.807511 -0.082151

31 6 0 -5.160857 -4.155937 -0.121197

32 6 0 -4.167592 -5.152964 -0.120998

33 6 0 -2.816546 -4.825170 -0.081479

34 6 0 -2.816546 4.825170 -0.081479

35 6 0 -4.167592 5.152964 -0.120998

36 6 0 -5.160857 4.155937 -0.121197

37 6 0 -4.818197 2.807511 -0.082151

38 6 0 4.818197 2.807511 -0.082151

39 6 0 5.160857 4.155937 -0.121197

40 6 0 4.167592 5.152964 -0.120998

41 6 0 2.816546 4.825170 -0.081479

42 1 0 5.581934 -2.036974 -0.085054

43 1 0 2.055429 -5.598283 -0.084079

44 1 0 -5.581934 -2.036974 -0.085054

45 1 0 -2.055429 -5.598283 -0.084079

46 1 0 -2.055429 5.598283 -0.084079

47 1 0 -5.581934 2.036974 -0.085054

48 1 0 5.581934 2.036974 -0.085054

49 1 0 2.055429 5.598283 -0.084079

50 1 0 -4.464352 6.196184 -0.153012

51 1 0 -6.205735 4.445688 -0.153339

52 1 0 4.464352 6.196184 -0.153012

53 1 0 6.205735 4.445688 -0.153339

54 1 0 6.205735 -4.445688 -0.153339

55 1 0 4.464352 -6.196184 -0.153012

56 1 0 -4.464352 -6.196184 -0.153012

57 1 0 -6.205735 -4.445688 -0.153339

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

Rotational constants (GHZ): 0.0881084 0.0879953 0.0441243

Leave Link 202 at Sat Jun 15 12:09:19 2019, MaxMem= 1342177280 cpu: 0.4

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 225 symmetry adapted cartesian basis functions of A1 symmetry.

There are 196 symmetry adapted cartesian basis functions of A2 symmetry.

There are 207 symmetry adapted cartesian basis functions of B1 symmetry.

There are 207 symmetry adapted cartesian basis functions of B2 symmetry.

There are 211 symmetry adapted basis functions of A1 symmetry.

There are 187 symmetry adapted basis functions of A2 symmetry.

There are 197 symmetry adapted basis functions of B1 symmetry.

There are 197 symmetry adapted basis functions of B2 symmetry.

792 basis functions, 1399 primitive gaussians, 835 cartesian basis functions

139 alpha electrons 138 beta electrons

nuclear repulsion energy 4375.5745292560 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= 57 NActive= 57 NUniq= 16 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1642878855 Hartrees.

Nuclear repulsion after empirical dispersion term = 4375.4102413704 Hartrees.

No density basis found on file 724.

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

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= 57.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 57

GePol: Total number of spheres = 57

GePol: Number of exposed spheres = 57 (100.00%)

GePol: Number of points = 4674

GePol: Average weight of points = 0.10

GePol: Minimum weight of points = 0.12D-08

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 348

GePol: Fraction of low-weight points (<1% of avg) = 7.45%

GePol: Cavity surface area = 485.253 Ang\*\*2

GePol: Cavity volume = 504.105 Ang\*\*3

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

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PCM non-electrostatic energy = -0.0144581783 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 4375.3957831921 Hartrees.

Leave Link 301 at Sat Jun 15 12:09:20 2019, MaxMem= 1342177280 cpu: 0.8

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 32896 NPrTT= 163506 LenC2= 22879 LenP2D= 61392.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 792 RedAO= T EigKep= 3.42D-05 NBF= 211 187 197 197

NBsUse= 792 1.00D-06 EigRej= -1.00D+00 NBFU= 211 187 197 197

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= 802 802 802 802 802 MxSgAt= 57 MxSgA2= 57.

Leave Link 302 at Sat Jun 15 12:09:21 2019, MaxMem= 1342177280 cpu: 14.3

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

DipDrv: MaxL=1.

Leave Link 303 at Sat Jun 15 12:09:22 2019, MaxMem= 1342177280 cpu: 3.3

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

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

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 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 (B2) (A1) (A2) (B1) (B2) (A1) (B1) (A1) (B1) (A2)

(A1) (B2) (A2) (B2) (B1) (A1) (A2) (B2) (B1) (A1)

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The electronic state of the initial guess is 2-B1.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7685 S= 0.5092

Generating alternative initial guess.

ExpMin= 3.51D-02 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -1733.84204742460

Leave Link 401 at Sat Jun 15 12:09:32 2019, MaxMem= 1342177280 cpu: 103.6

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 2129573 IEndB= 2129573 NGot= 1342177280 MDV= 1340762408

LenX= 1340762408 LenY= 1340064348

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= 560000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 65538828.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.66D-15 for 4660.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.31D-15 for 4665 3778.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.00D-15 for 4660.

Iteration 1 A^-1\*A deviation from orthogonality is 2.15D-08 for 1935 1916.

Iteration 2 A\*A^-1 deviation from unit magnitude is 3.77D-15 for 16.

Iteration 2 A\*A^-1 deviation from orthogonality is 4.31D-15 for 3404 1148.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 1120.

Iteration 2 A^-1\*A deviation from orthogonality is 4.44D-16 for 2690 2315.

E= -1733.50684949072

DIIS: error= 4.98D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1733.50684949072 IErMin= 1 ErrMin= 4.98D-04

ErrMax= 4.98D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.12D-03 BMatP= 1.12D-03

IDIUse=3 WtCom= 9.95D-01 WtEn= 4.98D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.368 Goal= None Shift= 0.000

Gap= 0.409 Goal= None Shift= 0.000

RMSDP=5.18D-05 MaxDP=1.63D-03 OVMax= 2.47D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 5.11D-05 CP: 1.00D+00

E= -1733.50716816977 Delta-E= -0.000318679049 Rises=F Damp=F

DIIS: error= 2.14D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1733.50716816977 IErMin= 2 ErrMin= 2.14D-04

ErrMax= 2.14D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.01D-04 BMatP= 1.12D-03

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.14D-03

Coeff-Com: 0.120D+00 0.880D+00

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

Coeff: 0.120D+00 0.880D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=1.32D-05 MaxDP=5.36D-04 DE=-3.19D-04 OVMax= 1.25D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.28D-05 CP: 1.00D+00 1.06D+00

E= -1733.50717543381 Delta-E= -0.000007264038 Rises=F Damp=F

DIIS: error= 2.29D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1733.50717543381 IErMin= 2 ErrMin= 2.14D-04

ErrMax= 2.29D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.07D-05 BMatP= 1.01D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.29D-03

Coeff-Com: -0.685D-02 0.471D+00 0.536D+00

Coeff-En: 0.000D+00 0.417D+00 0.583D+00

Coeff: -0.683D-02 0.471D+00 0.536D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=6.23D-06 MaxDP=2.41D-04 DE=-7.26D-06 OVMax= 9.84D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 3.72D-06 CP: 1.00D+00 1.05D+00 6.13D-01

E= -1733.50719275660 Delta-E= -0.000017322790 Rises=F Damp=F

DIIS: error= 9.18D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1733.50719275660 IErMin= 4 ErrMin= 9.18D-05

ErrMax= 9.18D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.18D-06 BMatP= 8.07D-05

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

Coeff-Com: -0.122D-01 0.226D+00 0.327D+00 0.459D+00

Coeff: -0.122D-01 0.226D+00 0.327D+00 0.459D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=1.87D-06 MaxDP=8.98D-05 DE=-1.73D-05 OVMax= 3.45D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.17D-06 CP: 1.00D+00 1.05D+00 6.21D-01 6.14D-01

E= -1733.50719486897 Delta-E= -0.000002112371 Rises=F Damp=F

DIIS: error= 1.61D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1733.50719486897 IErMin= 5 ErrMin= 1.61D-05

ErrMax= 1.61D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.21D-07 BMatP= 9.18D-06

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

Coeff-Com: -0.521D-02 0.657D-01 0.110D+00 0.223D+00 0.607D+00

Coeff: -0.521D-02 0.657D-01 0.110D+00 0.223D+00 0.607D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=5.06D-07 MaxDP=2.46D-05 DE=-2.11D-06 OVMax= 9.26D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 4.43D-07 CP: 1.00D+00 1.05D+00 6.12D-01 6.18D-01 8.66D-01

E= -1733.50719494192 Delta-E= -0.000000072952 Rises=F Damp=F

DIIS: error= 9.56D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1733.50719494192 IErMin= 6 ErrMin= 9.56D-06

ErrMax= 9.56D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.68D-08 BMatP= 4.21D-07

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

Coeff-Com: -0.679D-03-0.223D-02 0.541D-02 0.472D-01 0.345D+00 0.605D+00

Coeff: -0.679D-03-0.223D-02 0.541D-02 0.472D-01 0.345D+00 0.605D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=2.74D-07 MaxDP=1.23D-05 DE=-7.30D-08 OVMax= 4.27D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.52D-07 CP: 1.00D+00 1.05D+00 6.21D-01 6.25D-01 8.87D-01

CP: 6.69D-01

E= -1733.50719496152 Delta-E= -0.000000019592 Rises=F Damp=F

DIIS: error= 2.05D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1733.50719496152 IErMin= 7 ErrMin= 2.05D-06

ErrMax= 2.05D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.77D-09 BMatP= 8.68D-08

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

Coeff-Com: -0.206D-04-0.547D-02-0.455D-02 0.847D-02 0.127D+00 0.298D+00

Coeff-Com: 0.576D+00

Coeff: -0.206D-04-0.547D-02-0.455D-02 0.847D-02 0.127D+00 0.298D+00

Coeff: 0.576D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=8.18D-08 MaxDP=3.53D-06 DE=-1.96D-08 OVMax= 1.73D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 6.08D-08 CP: 1.00D+00 1.05D+00 6.20D-01 6.32D-01 9.02D-01

CP: 7.23D-01 7.67D-01

E= -1733.50719496334 Delta-E= -0.000000001828 Rises=F Damp=F

DIIS: error= 1.24D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1733.50719496334 IErMin= 8 ErrMin= 1.24D-06

ErrMax= 1.24D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.81D-09 BMatP= 6.77D-09

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

Coeff-Com: 0.140D-03-0.310D-02-0.429D-02-0.545D-02 0.475D-02 0.528D-01

Coeff-Com: 0.333D+00 0.622D+00

Coeff: 0.140D-03-0.310D-02-0.429D-02-0.545D-02 0.475D-02 0.528D-01

Coeff: 0.333D+00 0.622D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=4.24D-08 MaxDP=2.02D-06 DE=-1.83D-09 OVMax= 9.66D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 3.28D-08 CP: 1.00D+00 1.05D+00 6.20D-01 6.32D-01 9.08D-01

CP: 7.30D-01 9.23D-01 8.58D-01

E= -1733.50719496437 Delta-E= -0.000000001027 Rises=F Damp=F

DIIS: error= 5.52D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1733.50719496437 IErMin= 9 ErrMin= 5.52D-07

ErrMax= 5.52D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.95D-10 BMatP= 1.81D-09

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

Coeff-Com: 0.524D-04 0.490D-03-0.875D-04-0.408D-02-0.314D-01-0.626D-01

Coeff-Com: -0.610D-01 0.164D+00 0.995D+00

Coeff: 0.524D-04 0.490D-03-0.875D-04-0.408D-02-0.314D-01-0.626D-01

Coeff: -0.610D-01 0.164D+00 0.995D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=3.33D-08 MaxDP=1.64D-06 DE=-1.03D-09 OVMax= 8.78D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.79D-08 CP: 1.00D+00 1.05D+00 6.21D-01 6.32D-01 9.09D-01

CP: 7.42D-01 9.82D-01 1.27D+00 1.15D+00

E= -1733.50719496463 Delta-E= -0.000000000258 Rises=F Damp=F

DIIS: error= 4.57D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1733.50719496463 IErMin=10 ErrMin= 4.57D-07

ErrMax= 4.57D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.42D-10 BMatP= 2.95D-10

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

Coeff-Com: -0.148D-04 0.158D-02 0.161D-02-0.112D-02-0.259D-01-0.677D-01

Coeff-Com: -0.158D+00-0.991D-01 0.730D+00 0.620D+00

Coeff: -0.148D-04 0.158D-02 0.161D-02-0.112D-02-0.259D-01-0.677D-01

Coeff: -0.158D+00-0.991D-01 0.730D+00 0.620D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=2.14D-08 MaxDP=9.91D-07 DE=-2.58D-10 OVMax= 5.70D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 9.08D-09 CP: 1.00D+00 1.05D+00 6.20D-01 6.32D-01 9.12D-01

CP: 7.45D-01 1.04D+00 1.34D+00 1.63D+00 8.76D-01

E= -1733.50719496462 Delta-E= 0.000000000008 Rises=F Damp=F

DIIS: error= 1.50D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=10 EnMin= -1733.50719496463 IErMin=11 ErrMin= 1.50D-07

ErrMax= 1.50D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.51D-11 BMatP= 2.42D-10

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

Coeff-Com: -0.194D-04 0.202D-03 0.403D-03 0.985D-03 0.417D-02 0.434D-02

Coeff-Com: -0.901D-02-0.824D-01-0.175D+00 0.171D+00 0.108D+01

Coeff: -0.194D-04 0.202D-03 0.403D-03 0.985D-03 0.417D-02 0.434D-02

Coeff: -0.901D-02-0.824D-01-0.175D+00 0.171D+00 0.108D+01

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=1.20D-08 MaxDP=6.78D-07 DE= 8.19D-12 OVMax= 3.60D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 3.98D-09 CP: 1.00D+00 1.05D+00 6.20D-01 6.32D-01 9.11D-01

CP: 7.50D-01 1.06D+00 1.44D+00 1.80D+00 1.23D+00

CP: 1.24D+00

E= -1733.50719496458 Delta-E= 0.000000000040 Rises=F Damp=F

DIIS: error= 7.55D-08 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=10 EnMin= -1733.50719496463 IErMin=12 ErrMin= 7.55D-08

ErrMax= 7.55D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.75D-12 BMatP= 2.51D-11

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

Coeff-Com: -0.746D-05-0.927D-04-0.118D-05 0.606D-03 0.510D-02 0.101D-01

Coeff-Com: 0.136D-01-0.292D-01-0.174D+00 0.961D-02 0.543D+00 0.622D+00

Coeff: -0.746D-05-0.927D-04-0.118D-05 0.606D-03 0.510D-02 0.101D-01

Coeff: 0.136D-01-0.292D-01-0.174D+00 0.961D-02 0.543D+00 0.622D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=3.51D-09 MaxDP=1.74D-07 DE= 4.00D-11 OVMax= 9.54D-07

Error on total polarization charges = 0.07592

SCF Done: E(UB3LYP) = -1733.50719496 A.U. after 12 cycles

NFock= 12 Conv=0.35D-08 -V/T= 1.9757

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7682 S= 0.5091

<L.S>= 0.000000000000E+00

KE= 1.776720461796D+03 PE=-1.289798818767D+04 EE= 5.012364747719D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -9.07

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7682, after 0.7503

Leave Link 502 at Sat Jun 15 12:12:24 2019, MaxMem= 1342177280 cpu: 1964.3

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

Compute integral first derivatives.

... and contract with generalized density number 0.

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

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 32896 NPrTT= 163506 LenC2= 22879 LenP2D= 61392.

LDataN: DoStor=T MaxTD1= 6 Len= 172

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

GePol: Maximum number of non-zero 1st derivatives = 197

Leave Link 701 at Sat Jun 15 12:12:37 2019, MaxMem= 1342177280 cpu: 128.4

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

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

Leave Link 702 at Sat Jun 15 12:12:38 2019, MaxMem= 1342177280 cpu: 0.7

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

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=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= 800

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Sat Jun 15 12:12:57 2019, MaxMem= 1342177280 cpu: 220.9

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

Dipole =-4.51194637D-13-1.19015908D-13 8.48439286D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000213613 -0.000321012 -0.000125160

2 7 0.000156623 -0.000016311 0.000201353

3 6 -0.000301913 0.000106157 -0.000060191

4 6 0.000158717 0.000009966 -0.000029904

5 6 0.000158227 0.000250512 -0.000016985

6 7 0.000000000 -0.000571822 0.000085648

7 6 0.000301913 0.000106157 -0.000060191

8 7 -0.000156623 -0.000016311 0.000201353

9 6 0.000213613 -0.000321012 -0.000125160

10 6 -0.000158227 0.000250512 -0.000016985

11 6 -0.000158717 0.000009966 -0.000029904

12 7 -0.000504696 0.000000000 0.000136989

13 6 0.000158227 -0.000250512 -0.000016985

14 6 0.000158717 -0.000009966 -0.000029904

15 6 -0.000301913 -0.000106157 -0.000060191

16 7 0.000156623 0.000016311 0.000201353

17 6 -0.000213613 0.000321012 -0.000125160

18 7 0.000000000 0.000571822 0.000085648

19 7 -0.000156623 0.000016311 0.000201353

20 6 0.000301913 -0.000106157 -0.000060191

21 6 -0.000158717 -0.000009966 -0.000029904

22 6 -0.000158227 -0.000250512 -0.000016985

23 6 0.000213613 0.000321012 -0.000125160

24 7 0.000504696 0.000000000 0.000136989

25 30 0.000000000 0.000000000 -0.000123741

26 6 0.000181253 -0.000053702 -0.000018103

27 6 0.000374169 -0.000038786 -0.000012988

28 6 0.000028519 -0.000359430 -0.000013600

29 6 0.000059830 -0.000181563 -0.000024482

30 6 -0.000181253 -0.000053702 -0.000018103

31 6 -0.000374169 -0.000038786 -0.000012988

32 6 -0.000028519 -0.000359430 -0.000013600

33 6 -0.000059830 -0.000181563 -0.000024482

34 6 -0.000059830 0.000181563 -0.000024482

35 6 -0.000028519 0.000359430 -0.000013600

36 6 -0.000374169 0.000038786 -0.000012988

37 6 -0.000181253 0.000053702 -0.000018103

38 6 0.000181253 0.000053702 -0.000018103

39 6 0.000374169 0.000038786 -0.000012988

40 6 0.000028519 0.000359430 -0.000013600

41 6 0.000059830 0.000181563 -0.000024482

42 1 0.000035153 0.000129896 0.000008673

43 1 -0.000126218 -0.000041109 0.000009257

44 1 -0.000035153 0.000129896 0.000008673

45 1 0.000126218 -0.000041109 0.000009257

46 1 0.000126218 0.000041109 0.000009257

47 1 -0.000035153 -0.000129896 0.000008673

48 1 0.000035153 -0.000129896 0.000008673

49 1 -0.000126218 0.000041109 0.000009257

50 1 -0.000065053 0.000105522 0.000001746

51 1 -0.000103561 0.000064586 0.000000000

52 1 0.000065053 0.000105522 0.000001746

53 1 0.000103561 0.000064586 0.000000000

54 1 0.000103561 -0.000064586 0.000000000

55 1 0.000065053 -0.000105522 0.000001746

56 1 -0.000065053 -0.000105522 0.000001746

57 1 -0.000103561 -0.000064586 0.000000000

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

Cartesian Forces: Max 0.000571822 RMS 0.000165360

Leave Link 716 at Sat Jun 15 12:12:57 2019, MaxMem= 1342177280 cpu: 4.4

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

Internal Forces: Max 0.000763519 RMS 0.000169320

Search for a local minimum.

Step number 2 out of a maximum of 342

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

RMS Force = .16932D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 1 2

DE= -5.53D-04 DEPred=-6.20D-04 R= 8.92D-01

TightC=F SS= 1.41D+00 RLast= 6.10D-02 DXNew= 5.0454D-01 1.8307D-01

Trust test= 8.92D-01 RLast= 6.10D-02 DXMaxT set to 3.00D-01

ITU= 1 0

Use linear search instead of GDIIS.

Eigenvalues --- 0.01570 0.01587 0.01610 0.01610 0.01624

Eigenvalues --- 0.01645 0.01681 0.01697 0.01762 0.01767

Eigenvalues --- 0.01775 0.01780 0.01780 0.01782 0.01783

Eigenvalues --- 0.01788 0.01835 0.01846 0.01892 0.01895

Eigenvalues --- 0.01905 0.01958 0.01959 0.02008 0.02008

Eigenvalues --- 0.02008 0.02008 0.02051 0.02051 0.02051

Eigenvalues --- 0.02051 0.02053 0.02053 0.02053 0.02053

Eigenvalues --- 0.02077 0.02113 0.02113 0.02113 0.02113

Eigenvalues --- 0.02119 0.02119 0.02119 0.02119 0.02124

Eigenvalues --- 0.02124 0.02124 0.02124 0.02243 0.02249

Eigenvalues --- 0.02323 0.02331 0.03341 0.03920 0.03939

Eigenvalues --- 0.07479 0.15228 0.15973 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 0.16001 0.16256 0.16364

Eigenvalues --- 0.17348 0.22000 0.22000 0.22000 0.22000

Eigenvalues --- 0.22566 0.22598 0.22600 0.22600 0.24114

Eigenvalues --- 0.24298 0.24510 0.24510 0.24519 0.24529

Eigenvalues --- 0.24612 0.24618 0.24833 0.24948 0.24956

Eigenvalues --- 0.24985 0.24995 0.24997 0.24997 0.24998

Eigenvalues --- 0.25446 0.33725 0.34067 0.34312 0.34354

Eigenvalues --- 0.34800 0.34846 0.35155 0.35214 0.35218

Eigenvalues --- 0.35218 0.35218 0.35227 0.35243 0.35243

Eigenvalues --- 0.35243 0.35245 0.35247 0.35247 0.35247

Eigenvalues --- 0.35250 0.35252 0.35252 0.35252 0.35615

Eigenvalues --- 0.37367 0.37388 0.37564 0.38013 0.40798

Eigenvalues --- 0.40886 0.41928 0.41932 0.41947 0.41960

Eigenvalues --- 0.41970 0.42394 0.43207 0.43246 0.44575

Eigenvalues --- 0.45210 0.45216 0.45266 0.45342 0.45777

Eigenvalues --- 0.45910 0.45911 0.45918 0.46020 0.46122

Eigenvalues --- 0.46178 0.46179 0.46184 0.46689 0.48460

Eigenvalues --- 0.49756 0.50396 0.50600 0.51365 0.53527

Eigenvalues --- 0.55372 0.55378 0.55559 0.58008 0.58035

RFO step: Lambda=-1.76559293D-05 EMin= 1.57037402D-02

Quartic linear search produced a step of -0.09739.

Iteration 1 RMS(Cart)= 0.00241686 RMS(Int)= 0.00000093

Iteration 2 RMS(Cart)= 0.00000228 RMS(Int)= 0.00000025

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000025

ITry= 1 IFail=0 DXMaxC= 8.78D-03 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.27D-11 for atom 48.

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

(Linear) (Quad) (Total)

R1 2.56228 -0.00003 0.00053 -0.00072 -0.00019 2.56209

R2 2.76370 0.00076 0.00051 0.00133 0.00185 2.76555

R3 2.53736 0.00003 0.00066 -0.00061 0.00005 2.53741

R4 2.61915 0.00016 0.00040 -0.00022 0.00018 2.61933

R5 3.88213 0.00037 0.00053 0.00137 0.00190 3.88404

R6 2.74527 0.00068 0.00056 0.00104 0.00160 2.74687

R7 2.51302 0.00002 0.00064 -0.00060 0.00004 2.51307

R8 2.68023 0.00015 0.00059 -0.00026 0.00033 2.68056

R9 2.64004 0.00049 0.00073 0.00012 0.00085 2.64089

R10 2.63424 0.00048 0.00074 0.00009 0.00083 2.63507

R11 2.51302 0.00002 0.00064 -0.00060 0.00004 2.51307

R12 2.61915 0.00016 0.00040 -0.00022 0.00018 2.61933

R13 2.74527 0.00068 0.00056 0.00104 0.00160 2.74687

R14 2.56228 -0.00003 0.00053 -0.00072 -0.00019 2.56209

R15 3.88213 0.00037 0.00053 0.00137 0.00190 3.88404

R16 2.76370 0.00076 0.00051 0.00133 0.00185 2.76555

R17 2.53736 0.00003 0.00066 -0.00061 0.00005 2.53741

R18 2.68023 0.00015 0.00059 -0.00026 0.00033 2.68056

R19 2.63424 0.00048 0.00074 0.00009 0.00083 2.63507

R20 2.64004 0.00049 0.00073 0.00012 0.00085 2.64089

R21 2.53736 0.00003 0.00066 -0.00061 0.00005 2.53741

R22 2.68023 0.00015 0.00059 -0.00026 0.00033 2.68056

R23 2.76370 0.00076 0.00051 0.00133 0.00185 2.76555

R24 2.63424 0.00048 0.00074 0.00009 0.00083 2.63507

R25 2.74527 0.00068 0.00056 0.00104 0.00160 2.74687

R26 2.64004 0.00049 0.00073 0.00012 0.00085 2.64089

R27 2.61915 0.00016 0.00040 -0.00022 0.00018 2.61933

R28 2.51302 0.00002 0.00064 -0.00060 0.00004 2.51307

R29 2.56228 -0.00003 0.00053 -0.00072 -0.00019 2.56209

R30 3.88213 0.00037 0.00053 0.00137 0.00190 3.88404

R31 2.51302 0.00002 0.00064 -0.00060 0.00004 2.51307

R32 2.61915 0.00016 0.00040 -0.00022 0.00018 2.61933

R33 2.56228 -0.00003 0.00053 -0.00072 -0.00019 2.56209

R34 3.88213 0.00037 0.00053 0.00137 0.00190 3.88404

R35 2.74527 0.00068 0.00056 0.00104 0.00160 2.74687

R36 2.68023 0.00015 0.00059 -0.00026 0.00033 2.68056

R37 2.64004 0.00049 0.00073 0.00012 0.00085 2.64089

R38 2.76370 0.00076 0.00051 0.00133 0.00185 2.76555

R39 2.63424 0.00048 0.00074 0.00009 0.00083 2.63507

R40 2.53736 0.00003 0.00066 -0.00061 0.00005 2.53741

R41 2.63018 0.00040 0.00088 -0.00022 0.00066 2.63084

R42 2.05018 0.00012 0.00026 0.00000 0.00026 2.05044

R43 2.65951 0.00037 0.00078 -0.00012 0.00066 2.66017

R44 2.04995 0.00012 0.00027 -0.00001 0.00026 2.05021

R45 2.62824 0.00040 0.00089 -0.00024 0.00065 2.62889

R46 2.05050 0.00012 0.00027 0.00000 0.00026 2.05077

R47 2.05016 0.00012 0.00025 0.00001 0.00026 2.05043

R48 2.63018 0.00040 0.00088 -0.00022 0.00066 2.63084

R49 2.05018 0.00012 0.00026 0.00000 0.00026 2.05044

R50 2.65951 0.00037 0.00078 -0.00012 0.00066 2.66017

R51 2.04995 0.00012 0.00027 -0.00001 0.00026 2.05021

R52 2.62824 0.00040 0.00089 -0.00024 0.00065 2.62889

R53 2.05050 0.00012 0.00027 0.00000 0.00026 2.05077

R54 2.05016 0.00012 0.00025 0.00001 0.00026 2.05043

R55 2.62824 0.00040 0.00089 -0.00024 0.00065 2.62889

R56 2.05016 0.00012 0.00025 0.00001 0.00026 2.05043

R57 2.65951 0.00037 0.00078 -0.00012 0.00066 2.66017

R58 2.05050 0.00012 0.00027 0.00000 0.00026 2.05077

R59 2.63018 0.00040 0.00088 -0.00022 0.00066 2.63084

R60 2.04995 0.00012 0.00027 -0.00001 0.00026 2.05021

R61 2.05018 0.00012 0.00026 0.00000 0.00026 2.05044

R62 2.63018 0.00040 0.00088 -0.00022 0.00066 2.63084

R63 2.05018 0.00012 0.00026 0.00000 0.00026 2.05044

R64 2.65951 0.00037 0.00078 -0.00012 0.00066 2.66017

R65 2.04995 0.00012 0.00027 -0.00001 0.00026 2.05021

R66 2.62824 0.00040 0.00089 -0.00024 0.00065 2.62889

R67 2.05050 0.00012 0.00027 0.00000 0.00026 2.05077

R68 2.05016 0.00012 0.00025 0.00001 0.00026 2.05043

A1 1.88988 0.00013 0.00029 -0.00012 0.00017 1.89005

A2 2.23809 -0.00022 -0.00037 -0.00032 -0.00069 2.23740

A3 2.15516 0.00010 0.00008 0.00044 0.00052 2.15569

A4 1.92882 -0.00002 -0.00034 0.00052 0.00018 1.92900

A5 2.17887 -0.00001 0.00014 -0.00013 0.00002 2.17889

A6 2.16228 0.00004 0.00010 0.00010 0.00020 2.16248

A7 1.88363 0.00008 0.00029 -0.00025 0.00004 1.88367

A8 2.22225 -0.00024 -0.00035 -0.00042 -0.00078 2.22148

A9 2.17719 0.00016 0.00006 0.00067 0.00073 2.17792

A10 1.86067 -0.00006 -0.00012 0.00003 -0.00008 1.86059

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A12 2.10142 -0.00007 0.00005 -0.00038 -0.00033 2.10109

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A16 2.20325 0.00043 0.00038 0.00131 0.00169 2.20494

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A20 1.92882 -0.00002 -0.00034 0.00052 0.00018 1.92900

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A28 2.11086 -0.00004 0.00004 -0.00025 -0.00021 2.11065

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A38 2.32108 0.00013 0.00007 0.00034 0.00041 2.32148

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A41 2.22225 -0.00024 -0.00035 -0.00042 -0.00078 2.22148

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D2 -2.96518 -0.00004 0.00035 -0.00220 -0.00185 -2.96703

D3 -3.12284 0.00001 -0.00031 0.00107 0.00076 -3.12208

D4 0.18755 -0.00004 0.00029 -0.00213 -0.00183 0.18571

D5 -0.00402 -0.00001 0.00013 -0.00073 -0.00060 -0.00462

D6 -3.14074 0.00000 0.00002 -0.00030 -0.00028 -3.14102

D7 3.12709 -0.00001 0.00018 -0.00081 -0.00062 3.12646

D8 -0.00964 0.00000 0.00007 -0.00037 -0.00030 -0.00994

D9 0.01957 0.00003 -0.00019 0.00161 0.00141 0.02098

D10 -3.10934 0.00003 -0.00026 0.00169 0.00143 -3.10791

D11 -0.00818 0.00000 0.00028 -0.00087 -0.00059 -0.00877

D12 3.11745 -0.00001 0.00033 -0.00152 -0.00119 3.11626

D13 2.96654 0.00004 -0.00032 0.00227 0.00195 2.96850

D14 -0.19101 0.00003 -0.00027 0.00162 0.00135 -0.18966

D15 -3.06143 0.00001 -0.00046 0.00197 0.00150 -3.05993

D16 -0.27015 0.00004 -0.00029 0.00191 0.00162 -0.26853

D17 -1.66765 0.00003 -0.00038 0.00196 0.00158 -1.66607

D18 0.27085 -0.00004 0.00026 -0.00168 -0.00142 0.26944

D19 3.06213 -0.00001 0.00044 -0.00174 -0.00130 3.06083

D20 1.66464 -0.00002 0.00035 -0.00169 -0.00134 1.66330

D21 0.00538 0.00000 -0.00019 0.00037 0.00019 0.00556

D22 3.13949 0.00000 -0.00004 0.00010 0.00006 3.13955

D23 -3.12077 0.00001 -0.00023 0.00101 0.00079 -3.11998

D24 0.01334 0.00001 -0.00008 0.00074 0.00066 0.01400

D25 -0.01002 -0.00002 0.00019 -0.00098 -0.00079 -0.01080

D26 3.11309 -0.00003 0.00025 -0.00174 -0.00149 3.11160

D27 -0.00088 0.00001 0.00003 0.00021 0.00024 -0.00064

D28 3.13652 0.00000 0.00013 -0.00016 -0.00003 3.13649

D29 -3.13613 0.00001 -0.00009 0.00043 0.00034 -3.13578

D30 0.00128 0.00000 0.00000 0.00006 0.00007 0.00134

D31 -3.13806 0.00000 -0.00013 0.00007 -0.00006 -3.13812

D32 0.00479 0.00000 -0.00012 0.00037 0.00025 0.00505

D33 -0.00478 0.00000 0.00003 -0.00022 -0.00020 -0.00498

D34 3.13807 0.00000 0.00004 0.00008 0.00012 3.13819

D35 3.13926 0.00000 0.00009 -0.00034 -0.00025 3.13901

D36 -0.00321 -0.00001 0.00009 -0.00053 -0.00044 -0.00365

D37 0.00311 0.00000 -0.00004 0.00015 0.00011 0.00322

D38 -3.13937 0.00000 -0.00003 -0.00005 -0.00008 -3.13944

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D42 0.19101 -0.00003 0.00027 -0.00162 -0.00135 0.18966

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D44 -2.96654 -0.00004 0.00032 -0.00227 -0.00195 -2.96850

D45 3.12077 -0.00001 0.00023 -0.00101 -0.00079 3.11998

D46 -0.01334 -0.00001 0.00008 -0.00074 -0.00066 -0.01400

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D51 2.96518 0.00004 -0.00035 0.00220 0.00185 2.96703

D52 -0.18755 0.00004 -0.00029 0.00213 0.00183 -0.18571

D53 -0.27085 0.00004 -0.00026 0.00168 0.00142 -0.26944

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D61 -3.12709 0.00001 -0.00018 0.00081 0.00062 -3.12646

D62 0.00964 0.00000 -0.00007 0.00037 0.00030 0.00994

D63 -0.01957 -0.00003 0.00019 -0.00161 -0.00141 -0.02098

D64 3.10934 -0.00003 0.00026 -0.00169 -0.00143 3.10791

D65 0.00088 -0.00001 -0.00003 -0.00021 -0.00024 0.00064

D66 3.13613 -0.00001 0.00009 -0.00043 -0.00034 3.13578

D67 -3.13652 0.00000 -0.00013 0.00016 0.00003 -3.13649

D68 -0.00128 0.00000 0.00000 -0.00006 -0.00007 -0.00134

D69 -3.13926 0.00000 -0.00009 0.00034 0.00025 -3.13901

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D71 -0.00311 0.00000 0.00004 -0.00015 -0.00011 -0.00322

D72 3.13937 0.00000 0.00003 0.00005 0.00008 3.13944

D73 3.13806 0.00000 0.00013 -0.00007 0.00006 3.13812

D74 -0.00479 0.00000 0.00012 -0.00037 -0.00025 -0.00505

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D76 -3.13807 0.00000 -0.00004 -0.00008 -0.00012 -3.13819

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D78 -0.01957 -0.00003 0.00019 -0.00161 -0.00141 -0.02098

D79 0.00088 -0.00001 -0.00003 -0.00021 -0.00024 0.00064

D80 3.13613 -0.00001 0.00009 -0.00043 -0.00034 3.13578

D81 -3.13652 0.00000 -0.00013 0.00016 0.00003 -3.13649

D82 -0.00128 0.00000 0.00000 -0.00006 -0.00007 -0.00134

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D84 0.00402 0.00001 -0.00013 0.00073 0.00060 0.00462

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D86 3.14074 0.00000 -0.00002 0.00030 0.00028 3.14102

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D90 0.00321 0.00001 -0.00009 0.00053 0.00044 0.00365

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D94 -0.01334 -0.00001 0.00008 -0.00074 -0.00066 -0.01400

D95 0.00478 0.00000 -0.00003 0.00022 0.00020 0.00498

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D102 0.19101 -0.00003 0.00027 -0.00162 -0.00135 0.18966

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D106 -0.00762 -0.00001 0.00026 -0.00100 -0.00074 -0.00836

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D108 2.96518 0.00004 -0.00035 0.00220 0.00185 2.96703

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D163 3.13834 -0.00001 -0.00001 -0.00029 -0.00029 3.13805

D164 -0.00199 0.00000 0.00001 0.00001 0.00002 -0.00197

D165 -0.00393 0.00000 0.00004 -0.00019 -0.00015 -0.00409

D166 3.13883 -0.00001 0.00000 -0.00022 -0.00022 3.13861

D167 3.13854 0.00000 0.00003 0.00001 0.00003 3.13857

D168 -0.00188 0.00000 -0.00001 -0.00003 -0.00003 -0.00191

D169 0.00039 0.00000 0.00000 0.00003 0.00002 0.00041

D170 -3.14047 0.00000 -0.00004 -0.00008 -0.00012 -3.14058

D171 3.14082 0.00000 0.00003 0.00006 0.00009 3.14091

D172 -0.00004 0.00000 0.00000 -0.00005 -0.00005 -0.00009

D173 0.00399 0.00000 -0.00003 0.00018 0.00015 0.00414

D174 -3.13886 0.00000 -0.00004 -0.00012 -0.00016 -3.13903

D175 -3.13834 0.00001 0.00001 0.00029 0.00029 -3.13805

D176 0.00199 0.00000 -0.00001 -0.00001 -0.00002 0.00197

D177 -0.00399 0.00000 0.00003 -0.00018 -0.00015 -0.00414

D178 3.13834 -0.00001 -0.00001 -0.00029 -0.00029 3.13805

D179 3.13886 0.00000 0.00004 0.00012 0.00016 3.13903

D180 -0.00199 0.00000 0.00001 0.00001 0.00002 -0.00197

D181 -0.00039 0.00000 0.00000 -0.00003 -0.00002 -0.00041

D182 -3.14082 0.00000 -0.00003 -0.00006 -0.00009 -3.14091

D183 3.14047 0.00000 0.00004 0.00008 0.00012 3.14058

D184 0.00004 0.00000 0.00000 0.00005 0.00005 0.00009

D185 0.00393 0.00000 -0.00004 0.00019 0.00015 0.00409

D186 -3.13854 0.00000 -0.00003 -0.00001 -0.00003 -3.13857

D187 -3.13883 0.00001 0.00000 0.00022 0.00022 -3.13861

D188 0.00188 0.00000 0.00001 0.00003 0.00003 0.00191

D189 -0.00393 0.00000 0.00004 -0.00019 -0.00015 -0.00409

D190 3.13883 -0.00001 0.00000 -0.00022 -0.00022 3.13861

D191 3.13854 0.00000 0.00003 0.00001 0.00003 3.13857

D192 -0.00188 0.00000 -0.00001 -0.00003 -0.00003 -0.00191

D193 0.00039 0.00000 0.00000 0.00003 0.00002 0.00041

D194 -3.14047 0.00000 -0.00004 -0.00008 -0.00012 -3.14058

D195 3.14082 0.00000 0.00003 0.00006 0.00009 3.14091

D196 -0.00004 0.00000 0.00000 -0.00005 -0.00005 -0.00009

D197 0.00399 0.00000 -0.00003 0.00018 0.00015 0.00414

D198 -3.13886 0.00000 -0.00004 -0.00012 -0.00016 -3.13903

D199 -3.13834 0.00001 0.00001 0.00029 0.00029 -3.13805

D200 0.00199 0.00000 -0.00001 -0.00001 -0.00002 0.00197

Item Value Threshold Converged?

Maximum Force 0.000764 0.000450 NO

RMS Force 0.000169 0.000300 YES

Maximum Displacement 0.008781 0.001800 NO

RMS Displacement 0.002416 0.001200 NO

Predicted change in Energy=-1.531747D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jun 15 12:13:00 2019, MaxMem= 1342177280 cpu: 23.5

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

Stoichiometry C32H16N8Zn(1-,2)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C32H16N4)]

Deg. of freedom 43

Full point group C2V NOp 4

RotChk: IX=0 Diff= 4.33D-17

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 2.772382 1.184648 0.008457

2 7 0 1.438057 1.422754 0.041297

3 6 0 1.186666 2.785477 0.009128

4 6 0 2.465285 3.475337 -0.036926

5 6 0 3.467595 2.471600 -0.038100

6 7 0 0.000000 3.385697 0.000207

7 6 0 -1.186666 2.785477 0.009128

8 7 0 -1.438057 1.422754 0.041297

9 6 0 -2.772382 1.184648 0.008457

10 6 0 -3.467595 2.471600 -0.038100

11 6 0 -2.465285 3.475337 -0.036926

12 7 0 3.404464 0.000000 0.003492

13 6 0 3.467595 -2.471600 -0.038100

14 6 0 2.465285 -3.475337 -0.036926

15 6 0 1.186666 -2.785477 0.009128

16 7 0 1.438057 -1.422754 0.041297

17 6 0 2.772382 -1.184648 0.008457

18 7 0 0.000000 -3.385697 0.000207

19 7 0 -1.438057 -1.422754 0.041297

20 6 0 -1.186666 -2.785477 0.009128

21 6 0 -2.465285 -3.475337 -0.036926

22 6 0 -3.467595 -2.471600 -0.038100

23 6 0 -2.772382 -1.184648 0.008457

24 7 0 -3.404464 0.000000 0.003492

25 30 0 0.000000 0.000000 0.404889

26 6 0 4.819796 -2.809016 -0.084046

27 6 0 5.162967 -4.157619 -0.124884

28 6 0 4.169472 -5.154910 -0.124841

29 6 0 2.818217 -4.826727 -0.083669

30 6 0 -4.819796 -2.809016 -0.084046

31 6 0 -5.162967 -4.157619 -0.124884

32 6 0 -4.169472 -5.154910 -0.124841

33 6 0 -2.818217 -4.826727 -0.083669

34 6 0 -2.818217 4.826727 -0.083669

35 6 0 -4.169472 5.154910 -0.124841

36 6 0 -5.162967 4.157619 -0.124884

37 6 0 -4.819796 2.809016 -0.084046

38 6 0 4.819796 2.809016 -0.084046

39 6 0 5.162967 4.157619 -0.124884

40 6 0 4.169472 5.154910 -0.124841

41 6 0 2.818217 4.826727 -0.083669

42 1 0 5.583268 -2.038022 -0.086778

43 1 0 2.056745 -5.599685 -0.086233

44 1 0 -5.583268 -2.038022 -0.086778

45 1 0 -2.056745 -5.599685 -0.086233

46 1 0 -2.056745 5.599685 -0.086233

47 1 0 -5.583268 2.038022 -0.086778

48 1 0 5.583268 2.038022 -0.086778

49 1 0 2.056745 5.599685 -0.086233

50 1 0 -4.466320 6.198210 -0.158151

51 1 0 -6.207941 4.447394 -0.158251

52 1 0 4.466320 6.198210 -0.158151

53 1 0 6.207941 4.447394 -0.158251

54 1 0 6.207941 -4.447394 -0.158251

55 1 0 4.466320 -6.198210 -0.158151

56 1 0 -4.466320 -6.198210 -0.158151

57 1 0 -6.207941 -4.447394 -0.158251

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

Rotational constants (GHZ): 0.0880404 0.0879268 0.0440926

Leave Link 202 at Sat Jun 15 12:13:01 2019, MaxMem= 1342177280 cpu: 0.5

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 225 symmetry adapted cartesian basis functions of A1 symmetry.

There are 196 symmetry adapted cartesian basis functions of A2 symmetry.

There are 207 symmetry adapted cartesian basis functions of B1 symmetry.

There are 207 symmetry adapted cartesian basis functions of B2 symmetry.

There are 211 symmetry adapted basis functions of A1 symmetry.

There are 187 symmetry adapted basis functions of A2 symmetry.

There are 197 symmetry adapted basis functions of B1 symmetry.

There are 197 symmetry adapted basis functions of B2 symmetry.

792 basis functions, 1399 primitive gaussians, 835 cartesian basis functions

139 alpha electrons 138 beta electrons

nuclear repulsion energy 4374.1508503224 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= 57 NActive= 57 NUniq= 16 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1642503273 Hartrees.

Nuclear repulsion after empirical dispersion term = 4373.9865999951 Hartrees.

No density basis found on file 724.

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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= 57.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 57

GePol: Total number of spheres = 57

GePol: Number of exposed spheres = 57 (100.00%)

GePol: Number of points = 4678

GePol: Average weight of points = 0.10

GePol: Minimum weight of points = 0.76D-10

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 352

GePol: Fraction of low-weight points (<1% of avg) = 7.52%

GePol: Cavity surface area = 485.605 Ang\*\*2

GePol: Cavity volume = 504.329 Ang\*\*3

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

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PCM non-electrostatic energy = -0.0144431087 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 4373.9721568865 Hartrees.

Leave Link 301 at Sat Jun 15 12:13:01 2019, MaxMem= 1342177280 cpu: 0.6

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 32896 NPrTT= 163506 LenC2= 22879 LenP2D= 61376.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 792 RedAO= T EigKep= 3.44D-05 NBF= 211 187 197 197

NBsUse= 792 1.00D-06 EigRej= -1.00D+00 NBFU= 211 187 197 197

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= 802 802 802 802 802 MxSgAt= 57 MxSgA2= 57.

Leave Link 302 at Sat Jun 15 12:13:02 2019, MaxMem= 1342177280 cpu: 12.4

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

DipDrv: MaxL=1.

Leave Link 303 at Sat Jun 15 12:13:02 2019, MaxMem= 1342177280 cpu: 1.9

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

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

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 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 (B2) (A1) (A2) (B1) (B2) (A1) (B1) (A1) (B1) (A2)

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The electronic state of the initial guess is 2-B1.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7682 S= 0.5091

Leave Link 401 at Sat Jun 15 12:13:09 2019, MaxMem= 1342177280 cpu: 73.3

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 2129573 IEndB= 2129573 NGot= 1342177280 MDV= 1340762408

LenX= 1340762408 LenY= 1340064348

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= 560000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 65651052.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.22D-15 for 4670.

Iteration 1 A\*A^-1 deviation from orthogonality is 8.22D-15 for 4670 3783.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.10D-15 for 4670.

Iteration 1 A^-1\*A deviation from orthogonality is 2.69D-12 for 3734 3724.

E= -1733.50718313904

DIIS: error= 1.57D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1733.50718313904 IErMin= 1 ErrMin= 1.57D-04

ErrMax= 1.57D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.97D-05 BMatP= 6.97D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.57D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.368 Goal= None Shift= 0.000

Gap= 0.409 Goal= None Shift= 0.000

RMSDP=1.09D-05 MaxDP=2.99D-04 OVMax= 8.99D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.08D-05 CP: 1.00D+00

E= -1733.50721210302 Delta-E= -0.000028963978 Rises=F Damp=F

DIIS: error= 4.05D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1733.50721210302 IErMin= 2 ErrMin= 4.05D-05

ErrMax= 4.05D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.89D-06 BMatP= 6.97D-05

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

Coeff-Com: -0.202D-01 0.102D+01

Coeff: -0.202D-01 0.102D+01

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=1.73D-06 MaxDP=7.47D-05 DE=-2.90D-05 OVMax= 2.00D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.71D-06 CP: 1.00D+00 1.02D+00

E= -1733.50721214503 Delta-E= -0.000000042019 Rises=F Damp=F

DIIS: error= 6.31D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1733.50721214503 IErMin= 2 ErrMin= 4.05D-05

ErrMax= 6.31D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.99D-06 BMatP= 1.89D-06

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

Coeff-Com: -0.340D-01 0.591D+00 0.443D+00

Coeff: -0.340D-01 0.591D+00 0.443D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=1.19D-06 MaxDP=5.98D-05 DE=-4.20D-08 OVMax= 1.60D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 7.85D-07 CP: 1.00D+00 1.05D+00 5.41D-01

E= -1733.50721273943 Delta-E= -0.000000594391 Rises=F Damp=F

DIIS: error= 1.79D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1733.50721273943 IErMin= 4 ErrMin= 1.79D-05

ErrMax= 1.79D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.69D-07 BMatP= 1.89D-06

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

Coeff-Com: -0.142D-01 0.187D+00 0.227D+00 0.600D+00

Coeff: -0.142D-01 0.187D+00 0.227D+00 0.600D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=3.80D-07 MaxDP=1.96D-05 DE=-5.94D-07 OVMax= 4.42D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.56D-07 CP: 1.00D+00 1.05D+00 6.04D-01 7.00D-01

E= -1733.50721277134 Delta-E= -0.000000031914 Rises=F Damp=F

DIIS: error= 6.23D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1733.50721277134 IErMin= 5 ErrMin= 6.23D-06

ErrMax= 6.23D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.22D-08 BMatP= 1.69D-07

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

Coeff-Com: -0.335D-02 0.301D-01 0.694D-01 0.320D+00 0.584D+00

Coeff: -0.335D-02 0.301D-01 0.694D-01 0.320D+00 0.584D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=1.19D-07 MaxDP=4.24D-06 DE=-3.19D-08 OVMax= 2.15D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 9.44D-08 CP: 1.00D+00 1.05D+00 6.10D-01 7.22D-01 7.37D-01

E= -1733.50721277560 Delta-E= -0.000000004257 Rises=F Damp=F

DIIS: error= 1.93D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1733.50721277560 IErMin= 6 ErrMin= 1.93D-06

ErrMax= 1.93D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.90D-09 BMatP= 2.22D-08

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

Coeff-Com: -0.129D-03-0.816D-02 0.885D-02 0.958D-01 0.318D+00 0.585D+00

Coeff: -0.129D-03-0.816D-02 0.885D-02 0.958D-01 0.318D+00 0.585D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=4.63D-08 MaxDP=2.50D-06 DE=-4.26D-09 OVMax= 1.01D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.51D-08 CP: 1.00D+00 1.05D+00 6.13D-01 7.53D-01 7.54D-01

CP: 7.05D-01

E= -1733.50721277598 Delta-E= -0.000000000387 Rises=F Damp=F

DIIS: error= 4.25D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1733.50721277598 IErMin= 7 ErrMin= 4.25D-07

ErrMax= 4.25D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.07D-10 BMatP= 2.90D-09

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

Coeff-Com: 0.323D-03-0.839D-02-0.313D-02 0.183D-01 0.115D+00 0.307D+00

Coeff-Com: 0.571D+00

Coeff: 0.323D-03-0.839D-02-0.313D-02 0.183D-01 0.115D+00 0.307D+00

Coeff: 0.571D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=1.17D-08 MaxDP=7.67D-07 DE=-3.87D-10 OVMax= 2.62D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 9.56D-09 CP: 1.00D+00 1.05D+00 6.14D-01 7.51D-01 7.66D-01

CP: 7.43D-01 8.33D-01

E= -1733.50721277631 Delta-E= -0.000000000326 Rises=F Damp=F

DIIS: error= 2.70D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1733.50721277631 IErMin= 8 ErrMin= 2.70D-07

ErrMax= 2.70D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.08D-11 BMatP= 3.07D-10

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

Coeff-Com: 0.172D-03-0.336D-02-0.264D-02-0.161D-02 0.217D-01 0.875D-01

Coeff-Com: 0.304D+00 0.595D+00

Coeff: 0.172D-03-0.336D-02-0.264D-02-0.161D-02 0.217D-01 0.875D-01

Coeff: 0.304D+00 0.595D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=5.76D-09 MaxDP=2.49D-07 DE=-3.26D-10 OVMax= 1.72D-06

Error on total polarization charges = 0.07593

SCF Done: E(UB3LYP) = -1733.50721278 A.U. after 8 cycles

NFock= 8 Conv=0.58D-08 -V/T= 1.9757

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7682 S= 0.5091

<L.S>= 0.000000000000E+00

KE= 1.776676988943D+03 PE=-1.289509720518D+04 EE= 5.010940846570D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -9.06

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7682, after 0.7503

Leave Link 502 at Sat Jun 15 12:15:10 2019, MaxMem= 1342177280 cpu: 1379.5

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

Compute integral first derivatives.

... and contract with generalized density number 0.

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

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 32896 NPrTT= 163506 LenC2= 22879 LenP2D= 61376.

LDataN: DoStor=T MaxTD1= 6 Len= 172

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

GePol: Maximum number of non-zero 1st derivatives = 197

Leave Link 701 at Sat Jun 15 12:15:20 2019, MaxMem= 1342177280 cpu: 105.8

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

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

Leave Link 702 at Sat Jun 15 12:15:23 2019, MaxMem= 1342177280 cpu: 1.7

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

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=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= 800

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Sat Jun 15 12:15:41 2019, MaxMem= 1342177280 cpu: 217.4

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

Dipole =-2.34479103D-13-5.68434189D-14 8.44082161D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000074499 -0.000255518 -0.000061691

2 7 0.000164742 0.000070164 0.000137124

3 6 -0.000222869 0.000130778 -0.000052901

4 6 0.000063309 -0.000052636 -0.000004968

5 6 0.000024070 0.000110536 -0.000024448

6 7 0.000000000 -0.000223664 0.000045359

7 6 0.000222869 0.000130778 -0.000052901

8 7 -0.000164742 0.000070164 0.000137124

9 6 0.000074499 -0.000255518 -0.000061691

10 6 -0.000024070 0.000110536 -0.000024448

11 6 -0.000063309 -0.000052636 -0.000004968

12 7 -0.000135114 0.000000000 0.000080324

13 6 0.000024070 -0.000110536 -0.000024448

14 6 0.000063309 0.000052636 -0.000004968

15 6 -0.000222869 -0.000130778 -0.000052901

16 7 0.000164742 -0.000070164 0.000137124

17 6 -0.000074499 0.000255518 -0.000061691

18 7 0.000000000 0.000223664 0.000045359

19 7 -0.000164742 -0.000070164 0.000137124

20 6 0.000222869 -0.000130778 -0.000052901

21 6 -0.000063309 0.000052636 -0.000004968

22 6 -0.000024070 -0.000110536 -0.000024448

23 6 0.000074499 0.000255518 -0.000061691

24 7 0.000135114 0.000000000 0.000080324

25 30 0.000000000 0.000000000 -0.000193837

26 6 0.000014091 -0.000040225 -0.000006406

27 6 0.000058872 0.000050444 -0.000001087

28 6 -0.000057768 -0.000057354 -0.000000296

29 6 0.000050825 -0.000031804 0.000000312

30 6 -0.000014091 -0.000040225 -0.000006406

31 6 -0.000058872 0.000050444 -0.000001087

32 6 0.000057768 -0.000057354 -0.000000296

33 6 -0.000050825 -0.000031804 0.000000312

34 6 -0.000050825 0.000031804 0.000000312

35 6 0.000057768 0.000057354 -0.000000296

36 6 -0.000058872 -0.000050444 -0.000001087

37 6 -0.000014091 0.000040225 -0.000006406

38 6 0.000014091 0.000040225 -0.000006406

39 6 0.000058872 -0.000050444 -0.000001087

40 6 -0.000057768 0.000057354 -0.000000296

41 6 0.000050825 0.000031804 0.000000312

42 1 0.000007498 0.000036305 0.000000651

43 1 -0.000033355 -0.000010082 -0.000000696

44 1 -0.000007498 0.000036305 0.000000651

45 1 0.000033355 -0.000010082 -0.000000696

46 1 0.000033355 0.000010082 -0.000000696

47 1 -0.000007498 -0.000036305 0.000000651

48 1 0.000007498 -0.000036305 0.000000651

49 1 -0.000033355 0.000010082 -0.000000696

50 1 -0.000001968 0.000009991 -0.000000738

51 1 -0.000009037 0.000002326 0.000000761

52 1 0.000001968 0.000009991 -0.000000738

53 1 0.000009037 0.000002326 0.000000761

54 1 0.000009037 -0.000002326 0.000000761

55 1 0.000001968 -0.000009991 -0.000000738

56 1 -0.000001968 -0.000009991 -0.000000738

57 1 -0.000009037 -0.000002326 0.000000761

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

Cartesian Forces: Max 0.000255518 RMS 0.000081498

Leave Link 716 at Sat Jun 15 12:15:43 2019, MaxMem= 1342177280 cpu: 5.2

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

Internal Forces: Max 0.000130808 RMS 0.000031821

Search for a local minimum.

Step number 3 out of a maximum of 342

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

RMS Force = .31821D-04 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= -1.78D-05 DEPred=-1.53D-05 R= 1.16D+00

TightC=F SS= 1.41D+00 RLast= 1.53D-02 DXNew= 5.0454D-01 4.5799D-02

Trust test= 1.16D+00 RLast= 1.53D-02 DXMaxT set to 3.00D-01

ITU= 1 1 0

Eigenvalues --- 0.01512 0.01572 0.01587 0.01609 0.01624

Eigenvalues --- 0.01645 0.01681 0.01697 0.01703 0.01761

Eigenvalues --- 0.01772 0.01775 0.01780 0.01780 0.01782

Eigenvalues --- 0.01787 0.01834 0.01846 0.01892 0.01894

Eigenvalues --- 0.01903 0.01958 0.01959 0.02008 0.02008

Eigenvalues --- 0.02008 0.02008 0.02051 0.02051 0.02051

Eigenvalues --- 0.02051 0.02053 0.02053 0.02053 0.02053

Eigenvalues --- 0.02077 0.02113 0.02113 0.02113 0.02113

Eigenvalues --- 0.02119 0.02119 0.02119 0.02119 0.02124

Eigenvalues --- 0.02124 0.02124 0.02124 0.02188 0.02249

Eigenvalues --- 0.02305 0.02323 0.03339 0.03920 0.03938

Eigenvalues --- 0.07488 0.15227 0.15765 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 0.16013 0.16259 0.16366

Eigenvalues --- 0.16791 0.22000 0.22000 0.22000 0.22000

Eigenvalues --- 0.22578 0.22598 0.22600 0.22600 0.24131

Eigenvalues --- 0.24270 0.24510 0.24510 0.24512 0.24529

Eigenvalues --- 0.24619 0.24624 0.24836 0.24885 0.24948

Eigenvalues --- 0.24956 0.24992 0.24997 0.24997 0.24997

Eigenvalues --- 0.25900 0.33727 0.34031 0.34069 0.34313

Eigenvalues --- 0.34804 0.34851 0.35184 0.35201 0.35218

Eigenvalues --- 0.35218 0.35218 0.35218 0.35241 0.35243

Eigenvalues --- 0.35243 0.35243 0.35245 0.35247 0.35247

Eigenvalues --- 0.35247 0.35252 0.35252 0.35252 0.35865

Eigenvalues --- 0.36254 0.37367 0.37388 0.37565 0.40802

Eigenvalues --- 0.40889 0.41930 0.41932 0.41947 0.41960

Eigenvalues --- 0.41972 0.42323 0.43207 0.43247 0.44577

Eigenvalues --- 0.44736 0.45211 0.45217 0.45343 0.45785

Eigenvalues --- 0.45910 0.45911 0.45919 0.45994 0.46122

Eigenvalues --- 0.46178 0.46180 0.46184 0.46700 0.46903

Eigenvalues --- 0.50021 0.50393 0.51367 0.52915 0.53527

Eigenvalues --- 0.55373 0.55380 0.55777 0.58011 0.58038

En-DIIS/RFO-DIIS IScMMF= 0 using points: 3 2

RFO step: Lambda=-8.52201928D-07.

NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=F DC= 1.78D-05 SmlDif= 1.00D-05

RMS Error= 0.8610503354D-04 NUsed= 2 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.19530 -0.19530

Iteration 1 RMS(Cart)= 0.00163864 RMS(Int)= 0.00000059

Iteration 2 RMS(Cart)= 0.00000174 RMS(Int)= 0.00000022

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000022

ITry= 1 IFail=0 DXMaxC= 7.05D-03 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.49D-11 for atom 57.

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

(Linear) (Quad) (Total)

R1 2.56209 -0.00008 -0.00004 -0.00021 -0.00024 2.56185

R2 2.76555 0.00013 0.00036 0.00016 0.00052 2.76608

R3 2.53741 -0.00010 0.00001 -0.00030 -0.00029 2.53712

R4 2.61933 0.00003 0.00003 0.00002 0.00006 2.61939

R5 3.88404 0.00003 0.00037 0.00017 0.00055 3.88458

R6 2.74687 0.00008 0.00031 0.00002 0.00034 2.74720

R7 2.51307 -0.00012 0.00001 -0.00032 -0.00031 2.51275

R8 2.68056 0.00000 0.00006 -0.00008 -0.00002 2.68054

R9 2.64089 0.00005 0.00017 -0.00002 0.00015 2.64104

R10 2.63507 0.00003 0.00016 -0.00007 0.00009 2.63516

R11 2.51307 -0.00012 0.00001 -0.00032 -0.00031 2.51275

R12 2.61933 0.00003 0.00003 0.00002 0.00006 2.61939

R13 2.74687 0.00008 0.00031 0.00002 0.00034 2.74720

R14 2.56209 -0.00008 -0.00004 -0.00021 -0.00024 2.56185

R15 3.88404 0.00003 0.00037 0.00017 0.00055 3.88458

R16 2.76555 0.00013 0.00036 0.00016 0.00052 2.76608

R17 2.53741 -0.00010 0.00001 -0.00030 -0.00029 2.53712

R18 2.68056 0.00000 0.00006 -0.00008 -0.00002 2.68054

R19 2.63507 0.00003 0.00016 -0.00007 0.00009 2.63516

R20 2.64089 0.00005 0.00017 -0.00002 0.00015 2.64104

R21 2.53741 -0.00010 0.00001 -0.00030 -0.00029 2.53712

R22 2.68056 0.00000 0.00006 -0.00008 -0.00002 2.68054

R23 2.76555 0.00013 0.00036 0.00016 0.00052 2.76608

R24 2.63507 0.00003 0.00016 -0.00007 0.00009 2.63516

R25 2.74687 0.00008 0.00031 0.00002 0.00034 2.74720

R26 2.64089 0.00005 0.00017 -0.00002 0.00015 2.64104

R27 2.61933 0.00003 0.00003 0.00002 0.00006 2.61939

R28 2.51307 -0.00012 0.00001 -0.00032 -0.00031 2.51275

R29 2.56209 -0.00008 -0.00004 -0.00021 -0.00024 2.56185

R30 3.88404 0.00003 0.00037 0.00017 0.00055 3.88458

R31 2.51307 -0.00012 0.00001 -0.00032 -0.00031 2.51275

R32 2.61933 0.00003 0.00003 0.00002 0.00006 2.61939

R33 2.56209 -0.00008 -0.00004 -0.00021 -0.00024 2.56185

R34 3.88404 0.00003 0.00037 0.00017 0.00055 3.88458

R35 2.74687 0.00008 0.00031 0.00002 0.00034 2.74720

R36 2.68056 0.00000 0.00006 -0.00008 -0.00002 2.68054

R37 2.64089 0.00005 0.00017 -0.00002 0.00015 2.64104

R38 2.76555 0.00013 0.00036 0.00016 0.00052 2.76608

R39 2.63507 0.00003 0.00016 -0.00007 0.00009 2.63516

R40 2.53741 -0.00010 0.00001 -0.00030 -0.00029 2.53712

R41 2.63084 0.00001 0.00013 -0.00010 0.00003 2.63087

R42 2.05044 0.00003 0.00005 0.00006 0.00011 2.05055

R43 2.66017 0.00009 0.00013 0.00011 0.00024 2.66041

R44 2.05021 0.00001 0.00005 -0.00002 0.00003 2.05024

R45 2.62889 0.00001 0.00013 -0.00012 0.00001 2.62889

R46 2.05077 0.00001 0.00005 -0.00002 0.00004 2.05080

R47 2.05043 0.00003 0.00005 0.00006 0.00011 2.05053

R48 2.63084 0.00001 0.00013 -0.00010 0.00003 2.63087

R49 2.05044 0.00003 0.00005 0.00006 0.00011 2.05055

R50 2.66017 0.00009 0.00013 0.00011 0.00024 2.66041

R51 2.05021 0.00001 0.00005 -0.00002 0.00003 2.05024

R52 2.62889 0.00001 0.00013 -0.00012 0.00001 2.62889

R53 2.05077 0.00001 0.00005 -0.00002 0.00004 2.05080

R54 2.05043 0.00003 0.00005 0.00006 0.00011 2.05053

R55 2.62889 0.00001 0.00013 -0.00012 0.00001 2.62889

R56 2.05043 0.00003 0.00005 0.00006 0.00011 2.05053

R57 2.66017 0.00009 0.00013 0.00011 0.00024 2.66041

R58 2.05077 0.00001 0.00005 -0.00002 0.00004 2.05080

R59 2.63084 0.00001 0.00013 -0.00010 0.00003 2.63087

R60 2.05021 0.00001 0.00005 -0.00002 0.00003 2.05024

R61 2.05044 0.00003 0.00005 0.00006 0.00011 2.05055

R62 2.63084 0.00001 0.00013 -0.00010 0.00003 2.63087

R63 2.05044 0.00003 0.00005 0.00006 0.00011 2.05055

R64 2.66017 0.00009 0.00013 0.00011 0.00024 2.66041

R65 2.05021 0.00001 0.00005 -0.00002 0.00003 2.05024

R66 2.62889 0.00001 0.00013 -0.00012 0.00001 2.62889

R67 2.05077 0.00001 0.00005 -0.00002 0.00004 2.05080

R68 2.05043 0.00003 0.00005 0.00006 0.00011 2.05053

A1 1.89005 -0.00003 0.00003 -0.00020 -0.00017 1.88988

A2 2.23740 0.00001 -0.00014 0.00021 0.00007 2.23747

A3 2.15569 0.00001 0.00010 -0.00001 0.00009 2.15578

A4 1.92900 0.00007 0.00004 0.00030 0.00034 1.92934

A5 2.17889 -0.00005 0.00000 -0.00009 -0.00009 2.17880

A6 2.16248 -0.00002 0.00004 0.00004 0.00007 2.16256

A7 1.88367 -0.00004 0.00001 -0.00023 -0.00022 1.88345

A8 2.22148 -0.00002 -0.00015 0.00006 -0.00010 2.22138

A9 2.17792 0.00006 0.00014 0.00017 0.00031 2.17822

A10 1.86059 0.00001 -0.00002 0.00008 0.00007 1.86065

A11 2.32148 0.00000 0.00008 -0.00009 -0.00001 2.32147

A12 2.10109 0.00000 -0.00006 0.00001 -0.00005 2.10104

A13 1.86144 -0.00001 -0.00006 0.00004 -0.00002 1.86142

A14 2.31108 0.00000 0.00010 -0.00008 0.00002 2.31111

A15 2.11065 0.00001 -0.00004 0.00004 0.00000 2.11065

A16 2.20494 0.00008 0.00033 0.00014 0.00047 2.20542

A17 2.22148 -0.00002 -0.00015 0.00006 -0.00010 2.22138

A18 2.17792 0.00006 0.00014 0.00017 0.00031 2.17822

A19 1.88367 -0.00004 0.00001 -0.00023 -0.00022 1.88345

A20 1.92900 0.00007 0.00004 0.00030 0.00034 1.92934

A21 2.16248 -0.00002 0.00004 0.00004 0.00007 2.16256

A22 2.17889 -0.00005 0.00000 -0.00009 -0.00009 2.17880

A23 1.89005 -0.00003 0.00003 -0.00020 -0.00017 1.88988

A24 2.23740 0.00001 -0.00014 0.00021 0.00007 2.23747

A25 2.15569 0.00001 0.00010 -0.00001 0.00009 2.15578

A26 1.86144 -0.00001 -0.00006 0.00004 -0.00002 1.86142

A27 2.31108 0.00000 0.00010 -0.00008 0.00002 2.31111

A28 2.11065 0.00001 -0.00004 0.00004 0.00000 2.11065

A29 1.86059 0.00001 -0.00002 0.00008 0.00007 1.86065

A30 2.32148 0.00000 0.00008 -0.00009 -0.00001 2.32147

A31 2.10109 0.00000 -0.00006 0.00001 -0.00005 2.10104

A32 2.16130 0.00006 0.00034 -0.00001 0.00033 2.16163

A33 1.86144 -0.00001 -0.00006 0.00004 -0.00002 1.86142

A34 2.11065 0.00001 -0.00004 0.00004 0.00000 2.11065

A35 2.31108 0.00000 0.00010 -0.00008 0.00002 2.31111

A36 1.86059 0.00001 -0.00002 0.00008 0.00007 1.86065

A37 2.10109 0.00000 -0.00006 0.00001 -0.00005 2.10104

A38 2.32148 0.00000 0.00008 -0.00009 -0.00001 2.32147

A39 1.88367 -0.00004 0.00001 -0.00023 -0.00022 1.88345

A40 2.17792 0.00006 0.00014 0.00017 0.00031 2.17822

A41 2.22148 -0.00002 -0.00015 0.00006 -0.00010 2.22138

A42 1.92900 0.00007 0.00004 0.00030 0.00034 1.92934

A43 2.16248 -0.00002 0.00004 0.00004 0.00007 2.16256

A44 2.17889 -0.00005 0.00000 -0.00009 -0.00009 2.17880

A45 2.15569 0.00001 0.00010 -0.00001 0.00009 2.15578

A46 2.23740 0.00001 -0.00014 0.00021 0.00007 2.23747

A47 1.89005 -0.00003 0.00003 -0.00020 -0.00017 1.88988

A48 2.20494 0.00008 0.00033 0.00014 0.00047 2.20542

A49 1.92900 0.00007 0.00004 0.00030 0.00034 1.92934

A50 2.16248 -0.00002 0.00004 0.00004 0.00007 2.16256

A51 2.17889 -0.00005 0.00000 -0.00009 -0.00009 2.17880

A52 2.22148 -0.00002 -0.00015 0.00006 -0.00010 2.22138

A53 2.17792 0.00006 0.00014 0.00017 0.00031 2.17822

A54 1.88367 -0.00004 0.00001 -0.00023 -0.00022 1.88345

A55 1.86059 0.00001 -0.00002 0.00008 0.00007 1.86065

A56 2.32148 0.00000 0.00008 -0.00009 -0.00001 2.32147

A57 2.10109 0.00000 -0.00006 0.00001 -0.00005 2.10104

A58 1.86144 -0.00001 -0.00006 0.00004 -0.00002 1.86142

A59 2.11065 0.00001 -0.00004 0.00004 0.00000 2.11065

A60 2.31108 0.00000 0.00010 -0.00008 0.00002 2.31111

A61 1.89005 -0.00003 0.00003 -0.00020 -0.00017 1.88988

A62 2.23740 0.00001 -0.00014 0.00021 0.00007 2.23747

A63 2.15569 0.00001 0.00010 -0.00001 0.00009 2.15578

A64 2.16130 0.00006 0.00034 -0.00001 0.00033 2.16163

A65 1.54986 -0.00001 -0.00002 0.00001 -0.00001 1.54985

A66 1.52913 0.00001 0.00003 0.00008 0.00010 1.52923

A67 2.78592 0.00001 0.00002 0.00025 0.00027 2.78619

A68 2.78592 0.00001 0.00002 0.00025 0.00027 2.78619

A69 1.52913 0.00001 0.00003 0.00008 0.00010 1.52923

A70 1.54986 -0.00001 -0.00002 0.00001 -0.00001 1.54985

A71 2.06508 0.00001 0.00011 -0.00002 0.00009 2.06517

A72 2.10653 -0.00003 -0.00013 -0.00010 -0.00023 2.10629

A73 2.11157 0.00002 0.00002 0.00012 0.00015 2.11172

A74 2.10867 -0.00001 -0.00006 0.00000 -0.00007 2.10860

A75 2.09100 0.00001 0.00007 -0.00003 0.00005 2.09105

A76 2.08352 0.00001 -0.00001 0.00003 0.00002 2.08354

A77 2.11576 -0.00001 -0.00005 0.00000 -0.00006 2.11570

A78 2.08063 0.00001 -0.00001 0.00003 0.00002 2.08066

A79 2.08679 0.00000 0.00007 -0.00003 0.00004 2.08682

A80 2.06510 0.00001 0.00011 -0.00002 0.00010 2.06519

A81 2.10798 -0.00002 -0.00013 -0.00008 -0.00021 2.10777

A82 2.11010 0.00001 0.00001 0.00010 0.00011 2.11022

A83 2.06508 0.00001 0.00011 -0.00002 0.00009 2.06517

A84 2.10653 -0.00003 -0.00013 -0.00010 -0.00023 2.10629

A85 2.11157 0.00002 0.00002 0.00012 0.00015 2.11172

A86 2.10867 -0.00001 -0.00006 0.00000 -0.00007 2.10860

A87 2.09100 0.00001 0.00007 -0.00003 0.00005 2.09105

A88 2.08352 0.00001 -0.00001 0.00003 0.00002 2.08354

A89 2.11576 -0.00001 -0.00005 0.00000 -0.00006 2.11570

A90 2.08063 0.00001 -0.00001 0.00003 0.00002 2.08066

A91 2.08679 0.00000 0.00007 -0.00003 0.00004 2.08682

A92 2.06510 0.00001 0.00011 -0.00002 0.00010 2.06519

A93 2.10798 -0.00002 -0.00013 -0.00008 -0.00021 2.10777

A94 2.11010 0.00001 0.00001 0.00010 0.00011 2.11022

A95 2.06510 0.00001 0.00011 -0.00002 0.00010 2.06519

A96 2.10798 -0.00002 -0.00013 -0.00008 -0.00021 2.10777

A97 2.11010 0.00001 0.00001 0.00010 0.00011 2.11022

A98 2.11576 -0.00001 -0.00005 0.00000 -0.00006 2.11570

A99 2.08679 0.00000 0.00007 -0.00003 0.00004 2.08682

A100 2.08063 0.00001 -0.00001 0.00003 0.00002 2.08066

A101 2.10867 -0.00001 -0.00006 0.00000 -0.00007 2.10860

A102 2.08352 0.00001 -0.00001 0.00003 0.00002 2.08354

A103 2.09100 0.00001 0.00007 -0.00003 0.00005 2.09105

A104 2.06508 0.00001 0.00011 -0.00002 0.00009 2.06517

A105 2.10653 -0.00003 -0.00013 -0.00010 -0.00023 2.10629

A106 2.11157 0.00002 0.00002 0.00012 0.00015 2.11172

A107 2.06508 0.00001 0.00011 -0.00002 0.00009 2.06517

A108 2.10653 -0.00003 -0.00013 -0.00010 -0.00023 2.10629

A109 2.11157 0.00002 0.00002 0.00012 0.00015 2.11172

A110 2.10867 -0.00001 -0.00006 0.00000 -0.00007 2.10860

A111 2.09100 0.00001 0.00007 -0.00003 0.00005 2.09105

A112 2.08352 0.00001 -0.00001 0.00003 0.00002 2.08354

A113 2.11576 -0.00001 -0.00005 0.00000 -0.00006 2.11570

A114 2.08063 0.00001 -0.00001 0.00003 0.00002 2.08066

A115 2.08679 0.00000 0.00007 -0.00003 0.00004 2.08682

A116 2.06510 0.00001 0.00011 -0.00002 0.00010 2.06519

A117 2.10798 -0.00002 -0.00013 -0.00008 -0.00021 2.10777

A118 2.11010 0.00001 0.00001 0.00010 0.00011 2.11022

D1 0.00836 0.00000 0.00014 0.00022 0.00036 0.00872

D2 -2.96703 -0.00003 -0.00036 -0.00137 -0.00173 -2.96876

D3 -3.12208 0.00000 0.00015 0.00044 0.00059 -3.12150

D4 0.18571 -0.00002 -0.00036 -0.00114 -0.00150 0.18421

D5 -0.00462 0.00000 -0.00012 0.00003 -0.00009 -0.00471

D6 -3.14102 0.00000 -0.00005 0.00008 0.00003 -3.14099

D7 3.12646 0.00000 -0.00012 -0.00018 -0.00030 3.12616

D8 -0.00994 0.00000 -0.00006 -0.00013 -0.00019 -0.01013

D9 0.02098 0.00002 0.00028 0.00088 0.00115 0.02214

D10 -3.10791 0.00002 0.00028 0.00113 0.00141 -3.10649

D11 -0.00877 0.00000 -0.00011 -0.00037 -0.00049 -0.00925

D12 3.11626 0.00000 -0.00023 -0.00059 -0.00082 3.11544

D13 2.96850 0.00002 0.00038 0.00118 0.00156 2.97006

D14 -0.18966 0.00002 0.00026 0.00096 0.00123 -0.18843

D15 -3.05993 0.00001 0.00029 0.00077 0.00106 -3.05887

D16 -0.26853 0.00002 0.00032 0.00101 0.00132 -0.26721

D17 -1.66607 0.00002 0.00031 0.00089 0.00120 -1.66486

D18 0.26944 -0.00002 -0.00028 -0.00104 -0.00132 0.26812

D19 3.06083 -0.00001 -0.00025 -0.00081 -0.00106 3.05977

D20 1.66330 -0.00002 -0.00026 -0.00092 -0.00118 1.66212

D21 0.00556 0.00000 0.00004 0.00038 0.00041 0.00598

D22 3.13955 0.00000 0.00001 0.00008 0.00010 3.13965

D23 -3.11998 0.00001 0.00015 0.00059 0.00074 -3.11924

D24 0.01400 0.00000 0.00013 0.00030 0.00043 0.01443

D25 -0.01080 -0.00001 -0.00015 -0.00048 -0.00064 -0.01144

D26 3.11160 -0.00001 -0.00029 -0.00074 -0.00103 3.11057

D27 -0.00064 0.00000 0.00005 -0.00025 -0.00020 -0.00084

D28 3.13649 0.00000 -0.00001 -0.00029 -0.00030 3.13619

D29 -3.13578 0.00000 0.00007 0.00000 0.00007 -3.13572

D30 0.00134 0.00000 0.00001 -0.00004 -0.00003 0.00131

D31 -3.13812 0.00000 -0.00001 0.00031 0.00030 -3.13782

D32 0.00505 0.00000 0.00005 0.00019 0.00024 0.00528

D33 -0.00498 0.00000 -0.00004 -0.00001 -0.00005 -0.00503

D34 3.13819 0.00000 0.00002 -0.00014 -0.00012 3.13808

D35 3.13901 0.00000 -0.00005 0.00001 -0.00004 3.13898

D36 -0.00365 0.00000 -0.00009 -0.00001 -0.00010 -0.00374

D37 0.00322 0.00000 0.00002 0.00007 0.00009 0.00331

D38 -3.13944 0.00000 -0.00002 0.00005 0.00003 -3.13941

D39 0.01080 0.00001 0.00015 0.00048 0.00064 0.01144

D40 -3.11160 0.00001 0.00029 0.00074 0.00103 -3.11057

D41 -3.11626 0.00000 0.00023 0.00059 0.00082 -3.11544

D42 0.18966 -0.00002 -0.00026 -0.00096 -0.00123 0.18843

D43 0.00877 0.00000 0.00011 0.00037 0.00049 0.00925

D44 -2.96850 -0.00002 -0.00038 -0.00118 -0.00156 -2.97006

D45 3.11998 -0.00001 -0.00015 -0.00059 -0.00074 3.11924

D46 -0.01400 0.00000 -0.00013 -0.00030 -0.00043 -0.01443

D47 -0.00556 0.00000 -0.00004 -0.00038 -0.00041 -0.00598

D48 -3.13955 0.00000 -0.00001 -0.00008 -0.00010 -3.13965

D49 -0.00836 0.00000 -0.00014 -0.00022 -0.00036 -0.00872

D50 3.12208 0.00000 -0.00015 -0.00044 -0.00059 3.12150

D51 2.96703 0.00003 0.00036 0.00137 0.00173 2.96876

D52 -0.18571 0.00002 0.00036 0.00114 0.00150 -0.18421

D53 -0.26944 0.00002 0.00028 0.00104 0.00132 -0.26812

D54 -1.66330 0.00002 0.00026 0.00092 0.00118 -1.66212

D55 -3.06083 0.00001 0.00025 0.00081 0.00106 -3.05977

D56 3.05993 -0.00001 -0.00029 -0.00077 -0.00106 3.05887

D57 1.66607 -0.00002 -0.00031 -0.00089 -0.00120 1.66486

D58 0.26853 -0.00002 -0.00032 -0.00101 -0.00132 0.26721

D59 0.00462 0.00000 0.00012 -0.00003 0.00009 0.00471

D60 3.14102 0.00000 0.00005 -0.00008 -0.00003 3.14099

D61 -3.12646 0.00000 0.00012 0.00018 0.00030 -3.12616

D62 0.00994 0.00000 0.00006 0.00013 0.00019 0.01013

D63 -0.02098 -0.00002 -0.00028 -0.00088 -0.00115 -0.02214

D64 3.10791 -0.00002 -0.00028 -0.00113 -0.00141 3.10649

D65 0.00064 0.00000 -0.00005 0.00025 0.00020 0.00084

D66 3.13578 0.00000 -0.00007 0.00000 -0.00007 3.13572

D67 -3.13649 0.00000 0.00001 0.00029 0.00030 -3.13619

D68 -0.00134 0.00000 -0.00001 0.00004 0.00003 -0.00131

D69 -3.13901 0.00000 0.00005 -0.00001 0.00004 -3.13898

D70 0.00365 0.00000 0.00009 0.00001 0.00010 0.00374

D71 -0.00322 0.00000 -0.00002 -0.00007 -0.00009 -0.00331

D72 3.13944 0.00000 0.00002 -0.00005 -0.00003 3.13941

D73 3.13812 0.00000 0.00001 -0.00031 -0.00030 3.13782

D74 -0.00505 0.00000 -0.00005 -0.00019 -0.00024 -0.00528

D75 0.00498 0.00000 0.00004 0.00001 0.00005 0.00503

D76 -3.13819 0.00000 -0.00002 0.00014 0.00012 -3.13808

D77 3.10791 -0.00002 -0.00028 -0.00113 -0.00141 3.10649

D78 -0.02098 -0.00002 -0.00028 -0.00088 -0.00115 -0.02214

D79 0.00064 0.00000 -0.00005 0.00025 0.00020 0.00084

D80 3.13578 0.00000 -0.00007 0.00000 -0.00007 3.13572

D81 -3.13649 0.00000 0.00001 0.00029 0.00030 -3.13619

D82 -0.00134 0.00000 -0.00001 0.00004 0.00003 -0.00131

D83 -3.12646 0.00000 0.00012 0.00018 0.00030 -3.12616

D84 0.00462 0.00000 0.00012 -0.00003 0.00009 0.00471

D85 0.00994 0.00000 0.00006 0.00013 0.00019 0.01013

D86 3.14102 0.00000 0.00005 -0.00008 -0.00003 3.14099

D87 -0.00322 0.00000 -0.00002 -0.00007 -0.00009 -0.00331

D88 3.13944 0.00000 0.00002 -0.00005 -0.00003 3.13941

D89 -3.13901 0.00000 0.00005 -0.00001 0.00004 -3.13898

D90 0.00365 0.00000 0.00009 0.00001 0.00010 0.00374

D91 -0.00556 0.00000 -0.00004 -0.00038 -0.00041 -0.00598

D92 3.11998 -0.00001 -0.00015 -0.00059 -0.00074 3.11924

D93 -3.13955 0.00000 -0.00001 -0.00008 -0.00010 -3.13965

D94 -0.01400 0.00000 -0.00013 -0.00030 -0.00043 -0.01443

D95 0.00498 0.00000 0.00004 0.00001 0.00005 0.00503

D96 -3.13819 0.00000 -0.00002 0.00014 0.00012 -3.13808

D97 3.13812 0.00000 0.00001 -0.00031 -0.00030 3.13782

D98 -0.00505 0.00000 -0.00005 -0.00019 -0.00024 -0.00528

D99 0.00877 0.00000 0.00011 0.00037 0.00049 0.00925

D100 -2.96850 -0.00002 -0.00038 -0.00118 -0.00156 -2.97006

D101 -3.11626 0.00000 0.00023 0.00059 0.00082 -3.11544

D102 0.18966 -0.00002 -0.00026 -0.00096 -0.00123 0.18843

D103 -3.11160 0.00001 0.00029 0.00074 0.00103 -3.11057

D104 0.01080 0.00001 0.00015 0.00048 0.00064 0.01144

D105 3.12208 0.00000 -0.00015 -0.00044 -0.00059 3.12150

D106 -0.00836 0.00000 -0.00014 -0.00022 -0.00036 -0.00872

D107 -0.18571 0.00002 0.00036 0.00114 0.00150 -0.18421

D108 2.96703 0.00003 0.00036 0.00137 0.00173 2.96876

D109 -3.06083 0.00001 0.00025 0.00081 0.00106 -3.05977

D110 -1.66330 0.00002 0.00026 0.00092 0.00118 -1.66212

D111 -0.26944 0.00002 0.00028 0.00104 0.00132 -0.26812

D112 0.26853 -0.00002 -0.00032 -0.00101 -0.00132 0.26721

D113 1.66607 -0.00002 -0.00031 -0.00089 -0.00120 1.66486

D114 3.05993 -0.00001 -0.00029 -0.00077 -0.00106 3.05887

D115 -0.01080 -0.00001 -0.00015 -0.00048 -0.00064 -0.01144

D116 3.11160 -0.00001 -0.00029 -0.00074 -0.00103 3.11057

D117 3.11626 0.00000 -0.00023 -0.00059 -0.00082 3.11544

D118 -0.00877 0.00000 -0.00011 -0.00037 -0.00049 -0.00925

D119 -0.18966 0.00002 0.00026 0.00096 0.00123 -0.18843

D120 2.96850 0.00002 0.00038 0.00118 0.00156 2.97006

D121 0.00836 0.00000 0.00014 0.00022 0.00036 0.00872

D122 -3.12208 0.00000 0.00015 0.00044 0.00059 -3.12150

D123 -2.96703 -0.00003 -0.00036 -0.00137 -0.00173 -2.96876

D124 0.18571 -0.00002 -0.00036 -0.00114 -0.00150 0.18421

D125 1.66330 -0.00002 -0.00026 -0.00092 -0.00118 1.66212

D126 3.06083 -0.00001 -0.00025 -0.00081 -0.00106 3.05977

D127 0.26944 -0.00002 -0.00028 -0.00104 -0.00132 0.26812

D128 -1.66607 0.00002 0.00031 0.00089 0.00120 -1.66486

D129 -0.26853 0.00002 0.00032 0.00101 0.00132 -0.26721

D130 -3.05993 0.00001 0.00029 0.00077 0.00106 -3.05887

D131 -3.11998 0.00001 0.00015 0.00059 0.00074 -3.11924

D132 0.01400 0.00000 0.00013 0.00030 0.00043 0.01443

D133 0.00556 0.00000 0.00004 0.00038 0.00041 0.00598

D134 3.13955 0.00000 0.00001 0.00008 0.00010 3.13965

D135 -0.00064 0.00000 0.00005 -0.00025 -0.00020 -0.00084

D136 3.13649 0.00000 -0.00001 -0.00029 -0.00030 3.13619

D137 -3.13578 0.00000 0.00007 0.00000 0.00007 -3.13572

D138 0.00134 0.00000 0.00001 -0.00004 -0.00003 0.00131

D139 -3.13812 0.00000 -0.00001 0.00031 0.00030 -3.13782

D140 0.00505 0.00000 0.00005 0.00019 0.00024 0.00528

D141 -0.00498 0.00000 -0.00004 -0.00001 -0.00005 -0.00503

D142 3.13819 0.00000 0.00002 -0.00014 -0.00012 3.13808

D143 -0.00462 0.00000 -0.00012 0.00003 -0.00009 -0.00471

D144 3.12646 0.00000 -0.00012 -0.00018 -0.00030 3.12616

D145 -3.14102 0.00000 -0.00005 0.00008 0.00003 -3.14099

D146 -0.00994 0.00000 -0.00006 -0.00013 -0.00019 -0.01013

D147 0.00322 0.00000 0.00002 0.00007 0.00009 0.00331

D148 -3.13944 0.00000 -0.00002 0.00005 0.00003 -3.13941

D149 3.13901 0.00000 -0.00005 0.00001 -0.00004 3.13898

D150 -0.00365 0.00000 -0.00009 -0.00001 -0.00010 -0.00374

D151 0.02098 0.00002 0.00028 0.00088 0.00115 0.02214

D152 -3.10791 0.00002 0.00028 0.00113 0.00141 -3.10649

D153 0.00409 0.00000 0.00003 0.00005 0.00008 0.00417

D154 -3.13861 0.00000 0.00004 0.00003 0.00007 -3.13854

D155 -3.13857 0.00000 -0.00001 0.00002 0.00002 -3.13856

D156 0.00191 0.00000 0.00001 0.00000 0.00001 0.00192

D157 -0.00041 0.00000 0.00000 0.00000 0.00000 -0.00041

D158 3.14058 0.00000 0.00002 -0.00008 -0.00006 3.14053

D159 -3.14091 0.00000 -0.00002 0.00002 0.00001 -3.14090

D160 0.00009 0.00000 0.00001 -0.00006 -0.00005 0.00004

D161 -0.00414 0.00000 -0.00003 -0.00003 -0.00006 -0.00421

D162 3.13903 0.00000 0.00003 -0.00016 -0.00013 3.13890

D163 3.13805 0.00000 -0.00006 0.00005 -0.00001 3.13804

D164 -0.00197 0.00000 0.00000 -0.00008 -0.00007 -0.00204

D165 -0.00409 0.00000 -0.00003 -0.00005 -0.00008 -0.00417

D166 3.13861 0.00000 -0.00004 -0.00003 -0.00007 3.13854

D167 3.13857 0.00000 0.00001 -0.00002 -0.00002 3.13856

D168 -0.00191 0.00000 -0.00001 0.00000 -0.00001 -0.00192

D169 0.00041 0.00000 0.00000 0.00000 0.00000 0.00041

D170 -3.14058 0.00000 -0.00002 0.00008 0.00006 -3.14053

D171 3.14091 0.00000 0.00002 -0.00002 -0.00001 3.14090

D172 -0.00009 0.00000 -0.00001 0.00006 0.00005 -0.00004

D173 0.00414 0.00000 0.00003 0.00003 0.00006 0.00421

D174 -3.13903 0.00000 -0.00003 0.00016 0.00013 -3.13890

D175 -3.13805 0.00000 0.00006 -0.00005 0.00001 -3.13804

D176 0.00197 0.00000 0.00000 0.00008 0.00007 0.00204

D177 -0.00414 0.00000 -0.00003 -0.00003 -0.00006 -0.00421

D178 3.13805 0.00000 -0.00006 0.00005 -0.00001 3.13804

D179 3.13903 0.00000 0.00003 -0.00016 -0.00013 3.13890

D180 -0.00197 0.00000 0.00000 -0.00008 -0.00007 -0.00204

D181 -0.00041 0.00000 0.00000 0.00000 0.00000 -0.00041

D182 -3.14091 0.00000 -0.00002 0.00002 0.00001 -3.14090

D183 3.14058 0.00000 0.00002 -0.00008 -0.00006 3.14053

D184 0.00009 0.00000 0.00001 -0.00006 -0.00005 0.00004

D185 0.00409 0.00000 0.00003 0.00005 0.00008 0.00417

D186 -3.13857 0.00000 -0.00001 0.00002 0.00002 -3.13856

D187 -3.13861 0.00000 0.00004 0.00003 0.00007 -3.13854

D188 0.00191 0.00000 0.00001 0.00000 0.00001 0.00192

D189 -0.00409 0.00000 -0.00003 -0.00005 -0.00008 -0.00417

D190 3.13861 0.00000 -0.00004 -0.00003 -0.00007 3.13854

D191 3.13857 0.00000 0.00001 -0.00002 -0.00002 3.13856

D192 -0.00191 0.00000 -0.00001 0.00000 -0.00001 -0.00192

D193 0.00041 0.00000 0.00000 0.00000 0.00000 0.00041

D194 -3.14058 0.00000 -0.00002 0.00008 0.00006 -3.14053

D195 3.14091 0.00000 0.00002 -0.00002 -0.00001 3.14090

D196 -0.00009 0.00000 -0.00001 0.00006 0.00005 -0.00004

D197 0.00414 0.00000 0.00003 0.00003 0.00006 0.00421

D198 -3.13903 0.00000 -0.00003 0.00016 0.00013 -3.13890

D199 -3.13805 0.00000 0.00006 -0.00005 0.00001 -3.13804

D200 0.00197 0.00000 0.00000 0.00008 0.00007 0.00204

Item Value Threshold Converged?

Maximum Force 0.000131 0.000450 YES

RMS Force 0.000032 0.000300 YES

Maximum Displacement 0.007053 0.001800 NO

RMS Displacement 0.001639 0.001200 NO

Predicted change in Energy=-1.430943D-06

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jun 15 12:15:46 2019, MaxMem= 1342177280 cpu: 15.7

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

Stoichiometry C32H16N8Zn(1-,2)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C32H16N4)]

Deg. of freedom 43

Full point group C2V NOp 4

RotChk: IX=0 Diff= 3.74D-17

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 2.772362 1.184618 0.010082

2 7 0 1.438252 1.423032 0.044100

3 6 0 1.186660 2.785720 0.010687

4 6 0 2.465469 3.475502 -0.036865

5 6 0 3.467735 2.471737 -0.038181

6 7 0 0.000000 3.385581 0.001533

7 6 0 -1.186660 2.785720 0.010687

8 7 0 -1.438252 1.423032 0.044100

9 6 0 -2.772362 1.184618 0.010082

10 6 0 -3.467735 2.471737 -0.038181

11 6 0 -2.465469 3.475502 -0.036865

12 7 0 3.404179 0.000000 0.005141

13 6 0 3.467735 -2.471737 -0.038181

14 6 0 2.465469 -3.475502 -0.036865

15 6 0 1.186660 -2.785720 0.010687

16 7 0 1.438252 -1.423032 0.044100

17 6 0 2.772362 -1.184618 0.010082

18 7 0 0.000000 -3.385581 0.001533

19 7 0 -1.438252 -1.423032 0.044100

20 6 0 -1.186660 -2.785720 0.010687

21 6 0 -2.465469 -3.475502 -0.036865

22 6 0 -3.467735 -2.471737 -0.038181

23 6 0 -2.772362 -1.184618 0.010082

24 7 0 -3.404179 0.000000 0.005141

25 30 0 0.000000 0.000000 0.407466

26 6 0 4.819945 -2.809078 -0.085801

27 6 0 5.163240 -4.157621 -0.128059

28 6 0 4.169708 -5.155055 -0.127859

29 6 0 2.818493 -4.826897 -0.085118

30 6 0 -4.819945 -2.809078 -0.085801

31 6 0 -5.163240 -4.157621 -0.128059

32 6 0 -4.169708 -5.155055 -0.127859

33 6 0 -2.818493 -4.826897 -0.085118

34 6 0 -2.818493 4.826897 -0.085118

35 6 0 -4.169708 5.155055 -0.127859

36 6 0 -5.163240 4.157621 -0.128059

37 6 0 -4.819945 2.809078 -0.085801

38 6 0 4.819945 2.809078 -0.085801

39 6 0 5.163240 4.157621 -0.128059

40 6 0 4.169708 5.155055 -0.127859

41 6 0 2.818493 4.826897 -0.085118

42 1 0 5.583248 -2.037838 -0.088656

43 1 0 2.056885 -5.599800 -0.087685

44 1 0 -5.583248 -2.037838 -0.088656

45 1 0 -2.056885 -5.599800 -0.087685

46 1 0 -2.056885 5.599800 -0.087685

47 1 0 -5.583248 2.037838 -0.088656

48 1 0 5.583248 2.037838 -0.088656

49 1 0 2.056885 5.599800 -0.087685

50 1 0 -4.466560 6.198335 -0.162351

51 1 0 -6.208220 4.447297 -0.162673

52 1 0 4.466560 6.198335 -0.162351

53 1 0 6.208220 4.447297 -0.162673

54 1 0 6.208220 -4.447297 -0.162673

55 1 0 4.466560 -6.198335 -0.162351

56 1 0 -4.466560 -6.198335 -0.162351

57 1 0 -6.208220 -4.447297 -0.162673

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

Rotational constants (GHZ): 0.0880311 0.0879157 0.0440895

Leave Link 202 at Sat Jun 15 12:15:46 2019, MaxMem= 1342177280 cpu: 0.8

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 225 symmetry adapted cartesian basis functions of A1 symmetry.

There are 196 symmetry adapted cartesian basis functions of A2 symmetry.

There are 207 symmetry adapted cartesian basis functions of B1 symmetry.

There are 207 symmetry adapted cartesian basis functions of B2 symmetry.

There are 211 symmetry adapted basis functions of A1 symmetry.

There are 187 symmetry adapted basis functions of A2 symmetry.

There are 197 symmetry adapted basis functions of B1 symmetry.

There are 197 symmetry adapted basis functions of B2 symmetry.

792 basis functions, 1399 primitive gaussians, 835 cartesian basis functions

139 alpha electrons 138 beta electrons

nuclear repulsion energy 4373.9663799788 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= 57 NActive= 57 NUniq= 16 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1642464194 Hartrees.

Nuclear repulsion after empirical dispersion term = 4373.8021335593 Hartrees.

No density basis found on file 724.

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

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= 57.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 57

GePol: Total number of spheres = 57

GePol: Number of exposed spheres = 57 (100.00%)

GePol: Number of points = 4682

GePol: Average weight of points = 0.10

GePol: Minimum weight of points = 0.99D-09

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 364

GePol: Fraction of low-weight points (<1% of avg) = 7.77%

GePol: Cavity surface area = 485.735 Ang\*\*2

GePol: Cavity volume = 504.402 Ang\*\*3

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

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

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PCM non-electrostatic energy = -0.0144374419 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 4373.7876961174 Hartrees.

Leave Link 301 at Sat Jun 15 12:15:48 2019, MaxMem= 1342177280 cpu: 15.3

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 32896 NPrTT= 163506 LenC2= 22875 LenP2D= 61368.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 792 RedAO= T EigKep= 3.44D-05 NBF= 211 187 197 197

NBsUse= 792 1.00D-06 EigRej= -1.00D+00 NBFU= 211 187 197 197

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= 802 802 802 802 802 MxSgAt= 57 MxSgA2= 57.

Leave Link 302 at Sat Jun 15 12:15:51 2019, MaxMem= 1342177280 cpu: 15.9

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

DipDrv: MaxL=1.

Leave Link 303 at Sat Jun 15 12:15:51 2019, MaxMem= 1342177280 cpu: 1.6

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

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

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 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 (B2) (A1) (A2) (B1) (B2) (A1) (B1) (A1) (B1) (A2)

(A1) (B2) (A2) (B2) (B1) (A1) (A2) (B2) (B1) (A1)

(A2) (B1) (B2) (A1) (A2) (B1) (B2) (A1) (A2) (B2)

(B1) (A1) (A2) (B2) (B1) (A1) (A2) (B1) (B2) (A1)

(A1) (B2) (B1) (A2) (A1) (B2) (B1) (A1) (B2) (A2)

(B1) (A1) (A2) (B1) (B2) (A1) (A1) (B1) (B2) (A2)

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The electronic state of the initial guess is 2-B1.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7682 S= 0.5091

Leave Link 401 at Sat Jun 15 12:15:57 2019, MaxMem= 1342177280 cpu: 66.9

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 2129573 IEndB= 2129573 NGot= 1342177280 MDV= 1340762408

LenX= 1340762408 LenY= 1340064348

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= 560000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 65763372.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.99D-15 for 385.

Iteration 1 A\*A^-1 deviation from orthogonality is 6.42D-15 for 4674 3787.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.10D-15 for 780.

Iteration 1 A^-1\*A deviation from orthogonality is 2.00D-12 for 3873 3831.

E= -1733.50719689647

DIIS: error= 1.32D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1733.50719689647 IErMin= 1 ErrMin= 1.32D-04

ErrMax= 1.32D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.57D-05 BMatP= 3.57D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.32D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.368 Goal= None Shift= 0.000

Gap= 0.409 Goal= None Shift= 0.000

RMSDP=5.80D-06 MaxDP=1.15D-04 OVMax= 6.92D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 5.79D-06 CP: 1.00D+00

E= -1733.50721414533 Delta-E= -0.000017248861 Rises=F Damp=F

DIIS: error= 2.71D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1733.50721414533 IErMin= 2 ErrMin= 2.71D-05

ErrMax= 2.71D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.16D-07 BMatP= 3.57D-05

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

Coeff-Com: -0.486D-01 0.105D+01

Coeff: -0.486D-01 0.105D+01

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=1.36D-06 MaxDP=7.70D-05 DE=-1.72D-05 OVMax= 1.61D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.31D-06 CP: 1.00D+00 1.05D+00

E= -1733.50721415550 Delta-E= -0.000000010162 Rises=F Damp=F

DIIS: error= 5.71D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1733.50721415550 IErMin= 2 ErrMin= 2.71D-05

ErrMax= 5.71D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.60D-06 BMatP= 8.16D-07

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

Coeff-Com: -0.465D-01 0.646D+00 0.401D+00

Coeff: -0.465D-01 0.646D+00 0.401D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=9.27D-07 MaxDP=5.25D-05 DE=-1.02D-08 OVMax= 1.22D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 4.48D-07 CP: 1.00D+00 1.08D+00 4.09D-01

E= -1733.50721447544 Delta-E= -0.000000319948 Rises=F Damp=F

DIIS: error= 8.14D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1733.50721447544 IErMin= 4 ErrMin= 8.14D-06

ErrMax= 8.14D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.40D-08 BMatP= 8.16D-07

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

Coeff-Com: -0.104D-01 0.116D+00 0.165D+00 0.729D+00

Coeff: -0.104D-01 0.116D+00 0.165D+00 0.729D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=1.65D-07 MaxDP=7.07D-06 DE=-3.20D-07 OVMax= 2.59D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.31D-07 CP: 1.00D+00 1.08D+00 4.71D-01 8.76D-01

E= -1733.50721448383 Delta-E= -0.000000008391 Rises=F Damp=F

DIIS: error= 2.25D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1733.50721448383 IErMin= 5 ErrMin= 2.25D-06

ErrMax= 2.25D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.69D-09 BMatP= 4.40D-08

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

Coeff-Com: -0.209D-02 0.125D-01 0.603D-01 0.408D+00 0.521D+00

Coeff: -0.209D-02 0.125D-01 0.603D-01 0.408D+00 0.521D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=7.50D-08 MaxDP=3.77D-06 DE=-8.39D-09 OVMax= 1.60D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 5.03D-08 CP: 1.00D+00 1.08D+00 4.89D-01 8.94D-01 6.25D-01

E= -1733.50721448590 Delta-E= -0.000000002065 Rises=F Damp=F

DIIS: error= 6.63D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1733.50721448590 IErMin= 6 ErrMin= 6.63D-07

ErrMax= 6.63D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.66D-10 BMatP= 8.69D-09

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

Coeff-Com: 0.720D-03-0.167D-01 0.113D-02 0.858D-01 0.283D+00 0.646D+00

Coeff: 0.720D-03-0.167D-01 0.113D-02 0.858D-01 0.283D+00 0.646D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=2.27D-08 MaxDP=1.12D-06 DE=-2.07D-09 OVMax= 4.62D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.19D-08 CP: 1.00D+00 1.08D+00 4.87D-01 9.15D-01 6.85D-01

CP: 7.16D-01

E= -1733.50721448588 Delta-E= 0.000000000023 Rises=F Damp=F

DIIS: error= 3.59D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 6 EnMin= -1733.50721448590 IErMin= 7 ErrMin= 3.59D-07

ErrMax= 3.59D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.01D-11 BMatP= 9.66D-10

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

Coeff-Com: 0.480D-03-0.967D-02-0.195D-02 0.298D-01 0.133D+00 0.347D+00

Coeff-Com: 0.501D+00

Coeff: 0.480D-03-0.967D-02-0.195D-02 0.298D-01 0.133D+00 0.347D+00

Coeff: 0.501D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=7.35D-09 MaxDP=3.10D-07 DE= 2.27D-11 OVMax= 1.36D-06

Error on total polarization charges = 0.07593

SCF Done: E(UB3LYP) = -1733.50721449 A.U. after 7 cycles

NFock= 7 Conv=0.74D-08 -V/T= 1.9757

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7682 S= 0.5091

<L.S>= 0.000000000000E+00

KE= 1.776672915522D+03 PE=-1.289472316322D+04 EE= 5.010755337096D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -9.06

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7682, after 0.7503

Leave Link 502 at Sat Jun 15 12:17:46 2019, MaxMem= 1342177280 cpu: 1232.2

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

Compute integral first derivatives.

... and contract with generalized density number 0.

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

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 32896 NPrTT= 163506 LenC2= 22875 LenP2D= 61368.

LDataN: DoStor=T MaxTD1= 6 Len= 172

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

GePol: Maximum number of non-zero 1st derivatives = 197

Leave Link 701 at Sat Jun 15 12:17:55 2019, MaxMem= 1342177280 cpu: 104.2

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

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

Leave Link 702 at Sat Jun 15 12:17:56 2019, MaxMem= 1342177280 cpu: 3.3

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

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=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= 800

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Sat Jun 15 12:18:16 2019, MaxMem= 1342177280 cpu: 221.0

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

Dipole = 2.66453526D-13-2.84217094D-14 8.38647083D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000027824 -0.000012756 -0.000048814

2 7 0.000012906 -0.000013193 0.000093509

3 6 -0.000011169 0.000048747 -0.000021990

4 6 0.000022630 -0.000039864 -0.000009221

5 6 -0.000017905 0.000036754 0.000005216

6 7 0.000000000 -0.000033243 0.000019651

7 6 0.000011169 0.000048747 -0.000021990

8 7 -0.000012906 -0.000013193 0.000093509

9 6 0.000027824 -0.000012756 -0.000048814

10 6 0.000017905 0.000036754 0.000005216

11 6 -0.000022630 -0.000039864 -0.000009221

12 7 0.000018207 0.000000000 0.000037601

13 6 -0.000017905 -0.000036754 0.000005216

14 6 0.000022630 0.000039864 -0.000009221

15 6 -0.000011169 -0.000048747 -0.000021990

16 7 0.000012906 0.000013193 0.000093509

17 6 -0.000027824 0.000012756 -0.000048814

18 7 0.000000000 0.000033243 0.000019651

19 7 -0.000012906 0.000013193 0.000093509

20 6 0.000011169 -0.000048747 -0.000021990

21 6 -0.000022630 0.000039864 -0.000009221

22 6 0.000017905 -0.000036754 0.000005216

23 6 0.000027824 0.000012756 -0.000048814

24 7 -0.000018207 0.000000000 0.000037601

25 30 0.000000000 0.000000000 -0.000183749

26 6 -0.000002261 0.000002826 0.000002048

27 6 -0.000008908 0.000006513 0.000000096

28 6 -0.000008890 0.000010187 0.000000138

29 6 0.000000143 -0.000004436 -0.000003951

30 6 0.000002261 0.000002826 0.000002048

31 6 0.000008908 0.000006513 0.000000096

32 6 0.000008890 0.000010187 0.000000138

33 6 -0.000000143 -0.000004436 -0.000003951

34 6 -0.000000143 0.000004436 -0.000003951

35 6 0.000008890 -0.000010187 0.000000138

36 6 0.000008908 -0.000006513 0.000000096

37 6 0.000002261 -0.000002826 0.000002048

38 6 -0.000002261 -0.000002826 0.000002048

39 6 -0.000008908 -0.000006513 0.000000096

40 6 -0.000008890 -0.000010187 0.000000138

41 6 0.000000143 0.000004436 -0.000003951

42 1 -0.000002054 -0.000005568 -0.000001286

43 1 0.000004953 0.000002562 0.000000268

44 1 0.000002054 -0.000005568 -0.000001286

45 1 -0.000004953 0.000002562 0.000000268

46 1 -0.000004953 -0.000002562 0.000000268

47 1 0.000002054 0.000005568 -0.000001286

48 1 -0.000002054 0.000005568 -0.000001286

49 1 0.000004953 -0.000002562 0.000000268

50 1 0.000000659 -0.000004620 0.000001259

51 1 0.000004326 -0.000000610 0.000000039

52 1 -0.000000659 -0.000004620 0.000001259

53 1 -0.000004326 -0.000000610 0.000000039

54 1 -0.000004326 0.000000610 0.000000039

55 1 -0.000000659 0.000004620 0.000001259

56 1 0.000000659 0.000004620 0.000001259

57 1 0.000004326 0.000000610 0.000000039

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

Cartesian Forces: Max 0.000183749 RMS 0.000026403

Leave Link 716 at Sat Jun 15 12:18:18 2019, MaxMem= 1342177280 cpu: 12.8

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.000032578 RMS 0.000008660

Search for a local minimum.

Step number 4 out of a maximum of 342

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

RMS Force = .86599D-05 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 4

DE= -1.71D-06 DEPred=-1.43D-06 R= 1.19D+00

TightC=F SS= 1.41D+00 RLast= 1.04D-02 DXNew= 5.0454D-01 3.1224D-02

Trust test= 1.19D+00 RLast= 1.04D-02 DXMaxT set to 3.00D-01

ITU= 1 1 1 0

Eigenvalues --- 0.01128 0.01576 0.01586 0.01609 0.01624

Eigenvalues --- 0.01645 0.01667 0.01681 0.01697 0.01761

Eigenvalues --- 0.01772 0.01774 0.01779 0.01780 0.01782

Eigenvalues --- 0.01804 0.01834 0.01846 0.01892 0.01894

Eigenvalues --- 0.01923 0.01958 0.01959 0.02008 0.02008

Eigenvalues --- 0.02008 0.02009 0.02051 0.02051 0.02051

Eigenvalues --- 0.02051 0.02052 0.02053 0.02053 0.02053

Eigenvalues --- 0.02076 0.02110 0.02113 0.02113 0.02113

Eigenvalues --- 0.02113 0.02119 0.02119 0.02119 0.02124

Eigenvalues --- 0.02124 0.02124 0.02124 0.02128 0.02249

Eigenvalues --- 0.02299 0.02323 0.03338 0.03916 0.03934

Eigenvalues --- 0.07429 0.15227 0.15990 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 0.16028 0.16261 0.16367

Eigenvalues --- 0.17674 0.22000 0.22000 0.22000 0.22000

Eigenvalues --- 0.22598 0.22600 0.22600 0.22851 0.24145

Eigenvalues --- 0.24203 0.24511 0.24511 0.24512 0.24529

Eigenvalues --- 0.24625 0.24629 0.24761 0.24839 0.24948

Eigenvalues --- 0.24956 0.24993 0.24997 0.24997 0.24997

Eigenvalues --- 0.26067 0.33728 0.34070 0.34120 0.34313

Eigenvalues --- 0.34804 0.34851 0.35214 0.35218 0.35218

Eigenvalues --- 0.35218 0.35218 0.35243 0.35243 0.35243

Eigenvalues --- 0.35245 0.35247 0.35247 0.35247 0.35247

Eigenvalues --- 0.35252 0.35252 0.35252 0.35279 0.35660

Eigenvalues --- 0.37367 0.37388 0.37565 0.37881 0.40803

Eigenvalues --- 0.40890 0.41920 0.41932 0.41946 0.41959

Eigenvalues --- 0.41973 0.42585 0.43208 0.43247 0.44578

Eigenvalues --- 0.45042 0.45211 0.45217 0.45343 0.45862

Eigenvalues --- 0.45910 0.45911 0.45919 0.46025 0.46122

Eigenvalues --- 0.46178 0.46180 0.46184 0.46706 0.48326

Eigenvalues --- 0.49387 0.50393 0.51092 0.51369 0.53530

Eigenvalues --- 0.55373 0.55380 0.55508 0.58012 0.58038

En-DIIS/RFO-DIIS IScMMF= 0 using points: 4 3 2

RFO step: Lambda=-8.63227565D-08.

NNeg= 0 NP= 3 Switch= 2.50D-03 Rises=F DC= 1.78D-05 SmlDif= 1.00D-05

RMS Error= 0.3473985802D-04 NUsed= 3 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.32771 -0.36664 0.03892

Iteration 1 RMS(Cart)= 0.00062700 RMS(Int)= 0.00000012

Iteration 2 RMS(Cart)= 0.00000029 RMS(Int)= 0.00000008

ITry= 1 IFail=0 DXMaxC= 2.88D-03 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.84D-11 for atom 56.

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

(Linear) (Quad) (Total)

R1 2.56185 -0.00002 -0.00007 -0.00002 -0.00009 2.56175

R2 2.76608 0.00000 0.00010 0.00001 0.00011 2.76619

R3 2.53712 0.00000 -0.00010 0.00004 -0.00005 2.53707

R4 2.61939 0.00001 0.00001 0.00003 0.00004 2.61943

R5 3.88458 -0.00003 0.00011 -0.00017 -0.00006 3.88452

R6 2.74720 -0.00002 0.00005 -0.00003 0.00002 2.74722

R7 2.51275 -0.00002 -0.00010 0.00000 -0.00011 2.51265

R8 2.68054 -0.00003 -0.00002 -0.00009 -0.00011 2.68043

R9 2.64104 -0.00001 0.00002 0.00000 0.00001 2.64105

R10 2.63516 -0.00001 0.00000 0.00000 -0.00001 2.63515

R11 2.51275 -0.00002 -0.00010 0.00000 -0.00011 2.51265

R12 2.61939 0.00001 0.00001 0.00003 0.00004 2.61943

R13 2.74720 -0.00002 0.00005 -0.00003 0.00002 2.74722

R14 2.56185 -0.00002 -0.00007 -0.00002 -0.00009 2.56175

R15 3.88458 -0.00003 0.00011 -0.00017 -0.00006 3.88452

R16 2.76608 0.00000 0.00010 0.00001 0.00011 2.76619

R17 2.53712 0.00000 -0.00010 0.00004 -0.00005 2.53707

R18 2.68054 -0.00003 -0.00002 -0.00009 -0.00011 2.68043

R19 2.63516 -0.00001 0.00000 0.00000 -0.00001 2.63515

R20 2.64104 -0.00001 0.00002 0.00000 0.00001 2.64105

R21 2.53712 0.00000 -0.00010 0.00004 -0.00005 2.53707

R22 2.68054 -0.00003 -0.00002 -0.00009 -0.00011 2.68043

R23 2.76608 0.00000 0.00010 0.00001 0.00011 2.76619

R24 2.63516 -0.00001 0.00000 0.00000 -0.00001 2.63515

R25 2.74720 -0.00002 0.00005 -0.00003 0.00002 2.74722

R26 2.64104 -0.00001 0.00002 0.00000 0.00001 2.64105

R27 2.61939 0.00001 0.00001 0.00003 0.00004 2.61943

R28 2.51275 -0.00002 -0.00010 0.00000 -0.00011 2.51265

R29 2.56185 -0.00002 -0.00007 -0.00002 -0.00009 2.56175

R30 3.88458 -0.00003 0.00011 -0.00017 -0.00006 3.88452

R31 2.51275 -0.00002 -0.00010 0.00000 -0.00011 2.51265

R32 2.61939 0.00001 0.00001 0.00003 0.00004 2.61943

R33 2.56185 -0.00002 -0.00007 -0.00002 -0.00009 2.56175

R34 3.88458 -0.00003 0.00011 -0.00017 -0.00006 3.88452

R35 2.74720 -0.00002 0.00005 -0.00003 0.00002 2.74722

R36 2.68054 -0.00003 -0.00002 -0.00009 -0.00011 2.68043

R37 2.64104 -0.00001 0.00002 0.00000 0.00001 2.64105

R38 2.76608 0.00000 0.00010 0.00001 0.00011 2.76619

R39 2.63516 -0.00001 0.00000 0.00000 -0.00001 2.63515

R40 2.53712 0.00000 -0.00010 0.00004 -0.00005 2.53707

R41 2.63087 -0.00002 -0.00002 -0.00001 -0.00003 2.63084

R42 2.05055 -0.00001 0.00003 -0.00003 0.00000 2.05055

R43 2.66041 -0.00001 0.00005 -0.00004 0.00001 2.66042

R44 2.05024 0.00000 0.00000 -0.00001 -0.00001 2.05023

R45 2.62889 -0.00002 -0.00002 -0.00002 -0.00004 2.62885

R46 2.05080 0.00000 0.00000 -0.00001 -0.00001 2.05080

R47 2.05053 -0.00001 0.00002 -0.00003 0.00000 2.05053

R48 2.63087 -0.00002 -0.00002 -0.00001 -0.00003 2.63084

R49 2.05055 -0.00001 0.00003 -0.00003 0.00000 2.05055

R50 2.66041 -0.00001 0.00005 -0.00004 0.00001 2.66042

R51 2.05024 0.00000 0.00000 -0.00001 -0.00001 2.05023

R52 2.62889 -0.00002 -0.00002 -0.00002 -0.00004 2.62885

R53 2.05080 0.00000 0.00000 -0.00001 -0.00001 2.05080

R54 2.05053 -0.00001 0.00002 -0.00003 0.00000 2.05053

R55 2.62889 -0.00002 -0.00002 -0.00002 -0.00004 2.62885

R56 2.05053 -0.00001 0.00002 -0.00003 0.00000 2.05053

R57 2.66041 -0.00001 0.00005 -0.00004 0.00001 2.66042

R58 2.05080 0.00000 0.00000 -0.00001 -0.00001 2.05080

R59 2.63087 -0.00002 -0.00002 -0.00001 -0.00003 2.63084

R60 2.05024 0.00000 0.00000 -0.00001 -0.00001 2.05023

R61 2.05055 -0.00001 0.00003 -0.00003 0.00000 2.05055

R62 2.63087 -0.00002 -0.00002 -0.00001 -0.00003 2.63084

R63 2.05055 -0.00001 0.00003 -0.00003 0.00000 2.05055

R64 2.66041 -0.00001 0.00005 -0.00004 0.00001 2.66042

R65 2.05024 0.00000 0.00000 -0.00001 -0.00001 2.05023

R66 2.62889 -0.00002 -0.00002 -0.00002 -0.00004 2.62885

R67 2.05080 0.00000 0.00000 -0.00001 -0.00001 2.05080

R68 2.05053 -0.00001 0.00002 -0.00003 0.00000 2.05053

A1 1.88988 -0.00001 -0.00006 0.00002 -0.00004 1.88984

A2 2.23747 0.00001 0.00005 0.00000 0.00005 2.23752

A3 2.15578 0.00000 0.00001 -0.00001 0.00000 2.15578

A4 1.92934 0.00000 0.00010 -0.00005 0.00005 1.92939

A5 2.17880 0.00000 -0.00003 0.00006 0.00003 2.17882

A6 2.16256 0.00001 0.00002 0.00009 0.00011 2.16266

A7 1.88345 -0.00001 -0.00007 0.00002 -0.00006 1.88339

A8 2.22138 0.00000 0.00000 -0.00004 -0.00004 2.22134

A9 2.17822 0.00001 0.00007 0.00003 0.00010 2.17832

A10 1.86065 0.00001 0.00002 0.00001 0.00004 1.86069

A11 2.32147 -0.00001 -0.00002 -0.00002 -0.00004 2.32143

A12 2.10104 0.00000 0.00000 0.00001 0.00000 2.10104

A13 1.86142 0.00000 0.00001 0.00000 0.00000 1.86142

A14 2.31111 -0.00001 -0.00001 -0.00001 -0.00002 2.31109

A15 2.11065 0.00000 0.00001 0.00001 0.00001 2.11067

A16 2.20542 0.00000 0.00009 0.00003 0.00012 2.20554

A17 2.22138 0.00000 0.00000 -0.00004 -0.00004 2.22134

A18 2.17822 0.00001 0.00007 0.00003 0.00010 2.17832

A19 1.88345 -0.00001 -0.00007 0.00002 -0.00006 1.88339

A20 1.92934 0.00000 0.00010 -0.00005 0.00005 1.92939

A21 2.16256 0.00001 0.00002 0.00009 0.00011 2.16266

A22 2.17880 0.00000 -0.00003 0.00006 0.00003 2.17882

A23 1.88988 -0.00001 -0.00006 0.00002 -0.00004 1.88984

A24 2.23747 0.00001 0.00005 0.00000 0.00005 2.23752

A25 2.15578 0.00000 0.00001 -0.00001 0.00000 2.15578

A26 1.86142 0.00000 0.00001 0.00000 0.00000 1.86142

A27 2.31111 -0.00001 -0.00001 -0.00001 -0.00002 2.31109

A28 2.11065 0.00000 0.00001 0.00001 0.00001 2.11067

A29 1.86065 0.00001 0.00002 0.00001 0.00004 1.86069

A30 2.32147 -0.00001 -0.00002 -0.00002 -0.00004 2.32143

A31 2.10104 0.00000 0.00000 0.00001 0.00000 2.10104

A32 2.16163 -0.00001 0.00004 -0.00002 0.00002 2.16165

A33 1.86142 0.00000 0.00001 0.00000 0.00000 1.86142

A34 2.11065 0.00000 0.00001 0.00001 0.00001 2.11067

A35 2.31111 -0.00001 -0.00001 -0.00001 -0.00002 2.31109

A36 1.86065 0.00001 0.00002 0.00001 0.00004 1.86069

A37 2.10104 0.00000 0.00000 0.00001 0.00000 2.10104

A38 2.32147 -0.00001 -0.00002 -0.00002 -0.00004 2.32143

A39 1.88345 -0.00001 -0.00007 0.00002 -0.00006 1.88339

A40 2.17822 0.00001 0.00007 0.00003 0.00010 2.17832

A41 2.22138 0.00000 0.00000 -0.00004 -0.00004 2.22134

A42 1.92934 0.00000 0.00010 -0.00005 0.00005 1.92939

A43 2.16256 0.00001 0.00002 0.00009 0.00011 2.16266

A44 2.17880 0.00000 -0.00003 0.00006 0.00003 2.17882

A45 2.15578 0.00000 0.00001 -0.00001 0.00000 2.15578

A46 2.23747 0.00001 0.00005 0.00000 0.00005 2.23752

A47 1.88988 -0.00001 -0.00006 0.00002 -0.00004 1.88984

A48 2.20542 0.00000 0.00009 0.00003 0.00012 2.20554

A49 1.92934 0.00000 0.00010 -0.00005 0.00005 1.92939

A50 2.16256 0.00001 0.00002 0.00009 0.00011 2.16266

A51 2.17880 0.00000 -0.00003 0.00006 0.00003 2.17882

A52 2.22138 0.00000 0.00000 -0.00004 -0.00004 2.22134

A53 2.17822 0.00001 0.00007 0.00003 0.00010 2.17832

A54 1.88345 -0.00001 -0.00007 0.00002 -0.00006 1.88339

A55 1.86065 0.00001 0.00002 0.00001 0.00004 1.86069

A56 2.32147 -0.00001 -0.00002 -0.00002 -0.00004 2.32143

A57 2.10104 0.00000 0.00000 0.00001 0.00000 2.10104

A58 1.86142 0.00000 0.00001 0.00000 0.00000 1.86142

A59 2.11065 0.00000 0.00001 0.00001 0.00001 2.11067

A60 2.31111 -0.00001 -0.00001 -0.00001 -0.00002 2.31109

A61 1.88988 -0.00001 -0.00006 0.00002 -0.00004 1.88984

A62 2.23747 0.00001 0.00005 0.00000 0.00005 2.23752

A63 2.15578 0.00000 0.00001 -0.00001 0.00000 2.15578

A64 2.16163 -0.00001 0.00004 -0.00002 0.00002 2.16165

A65 1.54985 0.00000 0.00000 0.00005 0.00005 1.54990

A66 1.52923 0.00001 0.00003 0.00008 0.00011 1.52934

A67 2.78619 0.00002 0.00008 0.00038 0.00047 2.78666

A68 2.78619 0.00002 0.00008 0.00038 0.00047 2.78666

A69 1.52923 0.00001 0.00003 0.00008 0.00011 1.52934

A70 1.54985 0.00000 0.00000 0.00005 0.00005 1.54990

A71 2.06517 -0.00001 0.00001 -0.00001 0.00000 2.06517

A72 2.10629 0.00001 -0.00005 0.00003 -0.00002 2.10628

A73 2.11172 0.00000 0.00004 -0.00003 0.00002 2.11174

A74 2.10860 0.00000 -0.00001 0.00000 -0.00001 2.10859

A75 2.09105 0.00000 0.00000 0.00002 0.00002 2.09107

A76 2.08354 0.00000 0.00001 -0.00002 -0.00001 2.08353

A77 2.11570 0.00000 -0.00001 0.00000 -0.00001 2.11570

A78 2.08066 0.00000 0.00001 -0.00002 -0.00001 2.08064

A79 2.08682 0.00000 0.00000 0.00002 0.00002 2.08684

A80 2.06519 -0.00001 0.00001 -0.00001 0.00000 2.06519

A81 2.10777 0.00000 -0.00004 0.00002 -0.00002 2.10776

A82 2.11022 0.00000 0.00003 -0.00002 0.00002 2.11023

A83 2.06517 -0.00001 0.00001 -0.00001 0.00000 2.06517

A84 2.10629 0.00001 -0.00005 0.00003 -0.00002 2.10628

A85 2.11172 0.00000 0.00004 -0.00003 0.00002 2.11174

A86 2.10860 0.00000 -0.00001 0.00000 -0.00001 2.10859

A87 2.09105 0.00000 0.00000 0.00002 0.00002 2.09107

A88 2.08354 0.00000 0.00001 -0.00002 -0.00001 2.08353

A89 2.11570 0.00000 -0.00001 0.00000 -0.00001 2.11570

A90 2.08066 0.00000 0.00001 -0.00002 -0.00001 2.08064

A91 2.08682 0.00000 0.00000 0.00002 0.00002 2.08684

A92 2.06519 -0.00001 0.00001 -0.00001 0.00000 2.06519

A93 2.10777 0.00000 -0.00004 0.00002 -0.00002 2.10776

A94 2.11022 0.00000 0.00003 -0.00002 0.00002 2.11023

A95 2.06519 -0.00001 0.00001 -0.00001 0.00000 2.06519

A96 2.10777 0.00000 -0.00004 0.00002 -0.00002 2.10776

A97 2.11022 0.00000 0.00003 -0.00002 0.00002 2.11023

A98 2.11570 0.00000 -0.00001 0.00000 -0.00001 2.11570

A99 2.08682 0.00000 0.00000 0.00002 0.00002 2.08684

A100 2.08066 0.00000 0.00001 -0.00002 -0.00001 2.08064

A101 2.10860 0.00000 -0.00001 0.00000 -0.00001 2.10859

A102 2.08354 0.00000 0.00001 -0.00002 -0.00001 2.08353

A103 2.09105 0.00000 0.00000 0.00002 0.00002 2.09107

A104 2.06517 -0.00001 0.00001 -0.00001 0.00000 2.06517

A105 2.10629 0.00001 -0.00005 0.00003 -0.00002 2.10628

A106 2.11172 0.00000 0.00004 -0.00003 0.00002 2.11174

A107 2.06517 -0.00001 0.00001 -0.00001 0.00000 2.06517

A108 2.10629 0.00001 -0.00005 0.00003 -0.00002 2.10628

A109 2.11172 0.00000 0.00004 -0.00003 0.00002 2.11174

A110 2.10860 0.00000 -0.00001 0.00000 -0.00001 2.10859

A111 2.09105 0.00000 0.00000 0.00002 0.00002 2.09107

A112 2.08354 0.00000 0.00001 -0.00002 -0.00001 2.08353

A113 2.11570 0.00000 -0.00001 0.00000 -0.00001 2.11570

A114 2.08066 0.00000 0.00001 -0.00002 -0.00001 2.08064

A115 2.08682 0.00000 0.00000 0.00002 0.00002 2.08684

A116 2.06519 -0.00001 0.00001 -0.00001 0.00000 2.06519

A117 2.10777 0.00000 -0.00004 0.00002 -0.00002 2.10776

A118 2.11022 0.00000 0.00003 -0.00002 0.00002 2.11023

D1 0.00872 0.00000 0.00009 0.00035 0.00044 0.00915

D2 -2.96876 -0.00001 -0.00049 -0.00030 -0.00080 -2.96956

D3 -3.12150 0.00000 0.00016 0.00004 0.00020 -3.12129

D4 0.18421 -0.00002 -0.00042 -0.00061 -0.00103 0.18318

D5 -0.00471 0.00000 -0.00001 -0.00041 -0.00041 -0.00512

D6 -3.14099 0.00000 0.00002 -0.00021 -0.00019 -3.14118

D7 3.12616 0.00000 -0.00007 -0.00012 -0.00019 3.12597

D8 -0.01013 0.00000 -0.00005 0.00008 0.00003 -0.01010

D9 0.02214 0.00001 0.00032 0.00043 0.00076 0.02289

D10 -3.10649 0.00000 0.00041 0.00008 0.00049 -3.10601

D11 -0.00925 0.00000 -0.00014 -0.00015 -0.00029 -0.00954

D12 3.11544 0.00000 -0.00022 -0.00018 -0.00041 3.11504

D13 2.97006 0.00001 0.00044 0.00049 0.00092 2.97098

D14 -0.18843 0.00001 0.00035 0.00045 0.00080 -0.18763

D15 -3.05887 0.00000 0.00029 0.00018 0.00047 -3.05840

D16 -0.26721 0.00002 0.00037 0.00055 0.00092 -0.26629

D17 -1.66486 0.00001 0.00033 0.00037 0.00070 -1.66416

D18 0.26812 -0.00002 -0.00038 -0.00054 -0.00091 0.26720

D19 3.05977 0.00000 -0.00030 -0.00017 -0.00047 3.05930

D20 1.66212 -0.00001 -0.00033 -0.00035 -0.00068 1.66144

D21 0.00598 0.00000 0.00013 -0.00011 0.00002 0.00599

D22 3.13965 0.00000 0.00003 0.00000 0.00003 3.13968

D23 -3.11924 0.00000 0.00021 -0.00008 0.00013 -3.11911

D24 0.01443 0.00000 0.00011 0.00004 0.00015 0.01458

D25 -0.01144 0.00000 -0.00018 -0.00014 -0.00032 -0.01176

D26 3.11057 0.00000 -0.00028 -0.00018 -0.00046 3.11012

D27 -0.00084 0.00000 -0.00007 0.00031 0.00023 -0.00060

D28 3.13619 0.00000 -0.00010 0.00014 0.00004 3.13623

D29 -3.13572 0.00000 0.00001 0.00021 0.00022 -3.13549

D30 0.00131 0.00000 -0.00001 0.00004 0.00003 0.00134

D31 -3.13782 0.00000 0.00010 -0.00020 -0.00009 -3.13792

D32 0.00528 0.00000 0.00007 -0.00007 0.00000 0.00528

D33 -0.00503 0.00000 -0.00001 -0.00007 -0.00008 -0.00511

D34 3.13808 0.00000 -0.00004 0.00006 0.00001 3.13809

D35 3.13898 0.00000 0.00000 -0.00021 -0.00021 3.13876

D36 -0.00374 0.00000 -0.00001 -0.00015 -0.00016 -0.00390

D37 0.00331 0.00000 0.00003 0.00001 0.00004 0.00335

D38 -3.13941 0.00000 0.00001 0.00008 0.00009 -3.13932

D39 0.01144 0.00000 0.00018 0.00014 0.00032 0.01176

D40 -3.11057 0.00000 0.00028 0.00018 0.00046 -3.11012

D41 -3.11544 0.00000 0.00022 0.00018 0.00041 -3.11504

D42 0.18843 -0.00001 -0.00035 -0.00045 -0.00080 0.18763

D43 0.00925 0.00000 0.00014 0.00015 0.00029 0.00954

D44 -2.97006 -0.00001 -0.00044 -0.00049 -0.00092 -2.97098

D45 3.11924 0.00000 -0.00021 0.00008 -0.00013 3.11911

D46 -0.01443 0.00000 -0.00011 -0.00004 -0.00015 -0.01458

D47 -0.00598 0.00000 -0.00013 0.00011 -0.00002 -0.00599

D48 -3.13965 0.00000 -0.00003 0.00000 -0.00003 -3.13968

D49 -0.00872 0.00000 -0.00009 -0.00035 -0.00044 -0.00915

D50 3.12150 0.00000 -0.00016 -0.00004 -0.00020 3.12129

D51 2.96876 0.00001 0.00049 0.00030 0.00080 2.96956

D52 -0.18421 0.00002 0.00042 0.00061 0.00103 -0.18318

D53 -0.26812 0.00002 0.00038 0.00054 0.00091 -0.26720

D54 -1.66212 0.00001 0.00033 0.00035 0.00068 -1.66144

D55 -3.05977 0.00000 0.00030 0.00017 0.00047 -3.05930

D56 3.05887 0.00000 -0.00029 -0.00018 -0.00047 3.05840

D57 1.66486 -0.00001 -0.00033 -0.00037 -0.00070 1.66416

D58 0.26721 -0.00002 -0.00037 -0.00055 -0.00092 0.26629

D59 0.00471 0.00000 0.00001 0.00041 0.00041 0.00512

D60 3.14099 0.00000 -0.00002 0.00021 0.00019 3.14118

D61 -3.12616 0.00000 0.00007 0.00012 0.00019 -3.12597

D62 0.01013 0.00000 0.00005 -0.00008 -0.00003 0.01010

D63 -0.02214 -0.00001 -0.00032 -0.00043 -0.00076 -0.02289

D64 3.10649 0.00000 -0.00041 -0.00008 -0.00049 3.10601

D65 0.00084 0.00000 0.00007 -0.00031 -0.00023 0.00060

D66 3.13572 0.00000 -0.00001 -0.00021 -0.00022 3.13549

D67 -3.13619 0.00000 0.00010 -0.00014 -0.00004 -3.13623

D68 -0.00131 0.00000 0.00001 -0.00004 -0.00003 -0.00134

D69 -3.13898 0.00000 0.00000 0.00021 0.00021 -3.13876

D70 0.00374 0.00000 0.00001 0.00015 0.00016 0.00390

D71 -0.00331 0.00000 -0.00003 -0.00001 -0.00004 -0.00335

D72 3.13941 0.00000 -0.00001 -0.00008 -0.00009 3.13932

D73 3.13782 0.00000 -0.00010 0.00020 0.00009 3.13792

D74 -0.00528 0.00000 -0.00007 0.00007 0.00000 -0.00528

D75 0.00503 0.00000 0.00001 0.00007 0.00008 0.00511

D76 -3.13808 0.00000 0.00004 -0.00006 -0.00001 -3.13809

D77 3.10649 0.00000 -0.00041 -0.00008 -0.00049 3.10601

D78 -0.02214 -0.00001 -0.00032 -0.00043 -0.00076 -0.02289

D79 0.00084 0.00000 0.00007 -0.00031 -0.00023 0.00060

D80 3.13572 0.00000 -0.00001 -0.00021 -0.00022 3.13549

D81 -3.13619 0.00000 0.00010 -0.00014 -0.00004 -3.13623

D82 -0.00131 0.00000 0.00001 -0.00004 -0.00003 -0.00134

D83 -3.12616 0.00000 0.00007 0.00012 0.00019 -3.12597

D84 0.00471 0.00000 0.00001 0.00041 0.00041 0.00512

D85 0.01013 0.00000 0.00005 -0.00008 -0.00003 0.01010

D86 3.14099 0.00000 -0.00002 0.00021 0.00019 3.14118

D87 -0.00331 0.00000 -0.00003 -0.00001 -0.00004 -0.00335

D88 3.13941 0.00000 -0.00001 -0.00008 -0.00009 3.13932

D89 -3.13898 0.00000 0.00000 0.00021 0.00021 -3.13876

D90 0.00374 0.00000 0.00001 0.00015 0.00016 0.00390

D91 -0.00598 0.00000 -0.00013 0.00011 -0.00002 -0.00599

D92 3.11924 0.00000 -0.00021 0.00008 -0.00013 3.11911

D93 -3.13965 0.00000 -0.00003 0.00000 -0.00003 -3.13968

D94 -0.01443 0.00000 -0.00011 -0.00004 -0.00015 -0.01458

D95 0.00503 0.00000 0.00001 0.00007 0.00008 0.00511

D96 -3.13808 0.00000 0.00004 -0.00006 -0.00001 -3.13809

D97 3.13782 0.00000 -0.00010 0.00020 0.00009 3.13792

D98 -0.00528 0.00000 -0.00007 0.00007 0.00000 -0.00528

D99 0.00925 0.00000 0.00014 0.00015 0.00029 0.00954

D100 -2.97006 -0.00001 -0.00044 -0.00049 -0.00092 -2.97098

D101 -3.11544 0.00000 0.00022 0.00018 0.00041 -3.11504

D102 0.18843 -0.00001 -0.00035 -0.00045 -0.00080 0.18763

D103 -3.11057 0.00000 0.00028 0.00018 0.00046 -3.11012

D104 0.01144 0.00000 0.00018 0.00014 0.00032 0.01176

D105 3.12150 0.00000 -0.00016 -0.00004 -0.00020 3.12129

D106 -0.00872 0.00000 -0.00009 -0.00035 -0.00044 -0.00915

D107 -0.18421 0.00002 0.00042 0.00061 0.00103 -0.18318

D108 2.96876 0.00001 0.00049 0.00030 0.00080 2.96956

D109 -3.05977 0.00000 0.00030 0.00017 0.00047 -3.05930

D110 -1.66212 0.00001 0.00033 0.00035 0.00068 -1.66144

D111 -0.26812 0.00002 0.00038 0.00054 0.00091 -0.26720

D112 0.26721 -0.00002 -0.00037 -0.00055 -0.00092 0.26629

D113 1.66486 -0.00001 -0.00033 -0.00037 -0.00070 1.66416

D114 3.05887 0.00000 -0.00029 -0.00018 -0.00047 3.05840

D115 -0.01144 0.00000 -0.00018 -0.00014 -0.00032 -0.01176

D116 3.11057 0.00000 -0.00028 -0.00018 -0.00046 3.11012

D117 3.11544 0.00000 -0.00022 -0.00018 -0.00041 3.11504

D118 -0.00925 0.00000 -0.00014 -0.00015 -0.00029 -0.00954

D119 -0.18843 0.00001 0.00035 0.00045 0.00080 -0.18763

D120 2.97006 0.00001 0.00044 0.00049 0.00092 2.97098

D121 0.00872 0.00000 0.00009 0.00035 0.00044 0.00915

D122 -3.12150 0.00000 0.00016 0.00004 0.00020 -3.12129

D123 -2.96876 -0.00001 -0.00049 -0.00030 -0.00080 -2.96956

D124 0.18421 -0.00002 -0.00042 -0.00061 -0.00103 0.18318

D125 1.66212 -0.00001 -0.00033 -0.00035 -0.00068 1.66144

D126 3.05977 0.00000 -0.00030 -0.00017 -0.00047 3.05930

D127 0.26812 -0.00002 -0.00038 -0.00054 -0.00091 0.26720

D128 -1.66486 0.00001 0.00033 0.00037 0.00070 -1.66416

D129 -0.26721 0.00002 0.00037 0.00055 0.00092 -0.26629

D130 -3.05887 0.00000 0.00029 0.00018 0.00047 -3.05840

D131 -3.11924 0.00000 0.00021 -0.00008 0.00013 -3.11911

D132 0.01443 0.00000 0.00011 0.00004 0.00015 0.01458

D133 0.00598 0.00000 0.00013 -0.00011 0.00002 0.00599

D134 3.13965 0.00000 0.00003 0.00000 0.00003 3.13968

D135 -0.00084 0.00000 -0.00007 0.00031 0.00023 -0.00060

D136 3.13619 0.00000 -0.00010 0.00014 0.00004 3.13623

D137 -3.13572 0.00000 0.00001 0.00021 0.00022 -3.13549

D138 0.00131 0.00000 -0.00001 0.00004 0.00003 0.00134

D139 -3.13782 0.00000 0.00010 -0.00020 -0.00009 -3.13792

D140 0.00528 0.00000 0.00007 -0.00007 0.00000 0.00528

D141 -0.00503 0.00000 -0.00001 -0.00007 -0.00008 -0.00511

D142 3.13808 0.00000 -0.00004 0.00006 0.00001 3.13809

D143 -0.00471 0.00000 -0.00001 -0.00041 -0.00041 -0.00512

D144 3.12616 0.00000 -0.00007 -0.00012 -0.00019 3.12597

D145 -3.14099 0.00000 0.00002 -0.00021 -0.00019 -3.14118

D146 -0.01013 0.00000 -0.00005 0.00008 0.00003 -0.01010

D147 0.00331 0.00000 0.00003 0.00001 0.00004 0.00335

D148 -3.13941 0.00000 0.00001 0.00008 0.00009 -3.13932

D149 3.13898 0.00000 0.00000 -0.00021 -0.00021 3.13876

D150 -0.00374 0.00000 -0.00001 -0.00015 -0.00016 -0.00390

D151 0.02214 0.00001 0.00032 0.00043 0.00076 0.02289

D152 -3.10649 0.00000 0.00041 0.00008 0.00049 -3.10601

D153 0.00417 0.00000 0.00002 0.00003 0.00005 0.00422

D154 -3.13854 0.00000 0.00001 0.00000 0.00002 -3.13852

D155 -3.13856 0.00000 0.00001 0.00010 0.00010 -3.13845

D156 0.00192 0.00000 0.00000 0.00007 0.00007 0.00200

D157 -0.00041 0.00000 0.00000 0.00000 0.00000 -0.00041

D158 3.14053 0.00000 -0.00002 0.00004 0.00002 3.14054

D159 -3.14090 0.00000 0.00001 0.00003 0.00003 -3.14087

D160 0.00004 0.00000 -0.00002 0.00007 0.00005 0.00009

D161 -0.00421 0.00000 -0.00002 -0.00005 -0.00006 -0.00427

D162 3.13890 0.00000 -0.00005 0.00008 0.00003 3.13893

D163 3.13804 0.00000 0.00001 -0.00009 -0.00008 3.13796

D164 -0.00204 0.00000 -0.00002 0.00003 0.00001 -0.00203

D165 -0.00417 0.00000 -0.00002 -0.00003 -0.00005 -0.00422

D166 3.13854 0.00000 -0.00001 0.00000 -0.00002 3.13852

D167 3.13856 0.00000 -0.00001 -0.00010 -0.00010 3.13845

D168 -0.00192 0.00000 0.00000 -0.00007 -0.00007 -0.00200

D169 0.00041 0.00000 0.00000 0.00000 0.00000 0.00041

D170 -3.14053 0.00000 0.00002 -0.00004 -0.00002 -3.14054

D171 3.14090 0.00000 -0.00001 -0.00003 -0.00003 3.14087

D172 -0.00004 0.00000 0.00002 -0.00007 -0.00005 -0.00009

D173 0.00421 0.00000 0.00002 0.00005 0.00006 0.00427

D174 -3.13890 0.00000 0.00005 -0.00008 -0.00003 -3.13893

D175 -3.13804 0.00000 -0.00001 0.00009 0.00008 -3.13796

D176 0.00204 0.00000 0.00002 -0.00003 -0.00001 0.00203

D177 -0.00421 0.00000 -0.00002 -0.00005 -0.00006 -0.00427

D178 3.13804 0.00000 0.00001 -0.00009 -0.00008 3.13796

D179 3.13890 0.00000 -0.00005 0.00008 0.00003 3.13893

D180 -0.00204 0.00000 -0.00002 0.00003 0.00001 -0.00203

D181 -0.00041 0.00000 0.00000 0.00000 0.00000 -0.00041

D182 -3.14090 0.00000 0.00001 0.00003 0.00003 -3.14087

D183 3.14053 0.00000 -0.00002 0.00004 0.00002 3.14054

D184 0.00004 0.00000 -0.00002 0.00007 0.00005 0.00009

D185 0.00417 0.00000 0.00002 0.00003 0.00005 0.00422

D186 -3.13856 0.00000 0.00001 0.00010 0.00010 -3.13845

D187 -3.13854 0.00000 0.00001 0.00000 0.00002 -3.13852

D188 0.00192 0.00000 0.00000 0.00007 0.00007 0.00200

D189 -0.00417 0.00000 -0.00002 -0.00003 -0.00005 -0.00422

D190 3.13854 0.00000 -0.00001 0.00000 -0.00002 3.13852

D191 3.13856 0.00000 -0.00001 -0.00010 -0.00010 3.13845

D192 -0.00192 0.00000 0.00000 -0.00007 -0.00007 -0.00200

D193 0.00041 0.00000 0.00000 0.00000 0.00000 0.00041

D194 -3.14053 0.00000 0.00002 -0.00004 -0.00002 -3.14054

D195 3.14090 0.00000 -0.00001 -0.00003 -0.00003 3.14087

D196 -0.00004 0.00000 0.00002 -0.00007 -0.00005 -0.00009

D197 0.00421 0.00000 0.00002 0.00005 0.00006 0.00427

D198 -3.13890 0.00000 0.00005 -0.00008 -0.00003 -3.13893

D199 -3.13804 0.00000 -0.00001 0.00009 0.00008 -3.13796

D200 0.00204 0.00000 0.00002 -0.00003 -0.00001 0.00203

Item Value Threshold Converged?

Maximum Force 0.000033 0.000450 YES

RMS Force 0.000009 0.000300 YES

Maximum Displacement 0.002884 0.001800 NO

RMS Displacement 0.000627 0.001200 YES

Predicted change in Energy=-2.320375D-07

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jun 15 12:18:20 2019, MaxMem= 1342177280 cpu: 7.6

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

Stoichiometry C32H16N8Zn(1-,2)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C32H16N4)]

Deg. of freedom 43

Full point group C2V NOp 4

RotChk: IX=0 Diff= 7.43D-18

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 2.772294 1.184601 0.010690

2 7 0 1.438265 1.423092 0.045298

3 6 0 1.186646 2.785782 0.011266

4 6 0 2.465483 3.475486 -0.036964

5 6 0 3.467698 2.471751 -0.038060

6 7 0 0.000000 3.385545 0.001996

7 6 0 -1.186646 2.785782 0.011266

8 7 0 -1.438265 1.423092 0.045298

9 6 0 -2.772294 1.184601 0.010690

10 6 0 -3.467698 2.471751 -0.038060

11 6 0 -2.465483 3.475486 -0.036964

12 7 0 3.404086 0.000000 0.005849

13 6 0 3.467698 -2.471751 -0.038060

14 6 0 2.465483 -3.475486 -0.036964

15 6 0 1.186646 -2.785782 0.011266

16 7 0 1.438265 -1.423092 0.045298

17 6 0 2.772294 -1.184601 0.010690

18 7 0 0.000000 -3.385545 0.001996

19 7 0 -1.438265 -1.423092 0.045298

20 6 0 -1.186646 -2.785782 0.011266

21 6 0 -2.465483 -3.475486 -0.036964

22 6 0 -3.467698 -2.471751 -0.038060

23 6 0 -2.772294 -1.184601 0.010690

24 7 0 -3.404086 0.000000 0.005849

25 30 0 0.000000 0.000000 0.408186

26 6 0 4.819902 -2.809036 -0.086159

27 6 0 5.163218 -4.157537 -0.129072

28 6 0 4.169696 -5.154986 -0.129109

29 6 0 2.818507 -4.826862 -0.085957

30 6 0 -4.819902 -2.809036 -0.086159

31 6 0 -5.163218 -4.157537 -0.129072

32 6 0 -4.169696 -5.154986 -0.129109

33 6 0 -2.818507 -4.826862 -0.085957

34 6 0 -2.818507 4.826862 -0.085957

35 6 0 -4.169696 5.154986 -0.129109

36 6 0 -5.163218 4.157537 -0.129072

37 6 0 -4.819902 2.809036 -0.086159

38 6 0 4.819902 2.809036 -0.086159

39 6 0 5.163218 4.157537 -0.129072

40 6 0 4.169696 5.154986 -0.129109

41 6 0 2.818507 4.826862 -0.085957

42 1 0 5.583169 -2.037761 -0.088926

43 1 0 2.056891 -5.599756 -0.088682

44 1 0 -5.583169 -2.037761 -0.088926

45 1 0 -2.056891 -5.599756 -0.088682

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47 1 0 -5.583169 2.037761 -0.088926

48 1 0 5.583169 2.037761 -0.088926

49 1 0 2.056891 5.599756 -0.088682

50 1 0 -4.466566 6.198241 -0.164097

51 1 0 -6.208188 4.447190 -0.164051

52 1 0 4.466566 6.198241 -0.164097

53 1 0 6.208188 4.447190 -0.164051

54 1 0 6.208188 -4.447190 -0.164051

55 1 0 4.466566 -6.198241 -0.164097

56 1 0 -4.466566 -6.198241 -0.164097

57 1 0 -6.208188 -4.447190 -0.164051

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

Rotational constants (GHZ): 0.0880312 0.0879156 0.0440902

Leave Link 202 at Sat Jun 15 12:18:20 2019, MaxMem= 1342177280 cpu: 0.1

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 225 symmetry adapted cartesian basis functions of A1 symmetry.

There are 196 symmetry adapted cartesian basis functions of A2 symmetry.

There are 207 symmetry adapted cartesian basis functions of B1 symmetry.

There are 207 symmetry adapted cartesian basis functions of B2 symmetry.

There are 211 symmetry adapted basis functions of A1 symmetry.

There are 187 symmetry adapted basis functions of A2 symmetry.

There are 197 symmetry adapted basis functions of B1 symmetry.

There are 197 symmetry adapted basis functions of B2 symmetry.

792 basis functions, 1399 primitive gaussians, 835 cartesian basis functions

139 alpha electrons 138 beta electrons

nuclear repulsion energy 4373.9833173677 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= 57 NActive= 57 NUniq= 16 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1642463430 Hartrees.

Nuclear repulsion after empirical dispersion term = 4373.8190710248 Hartrees.

No density basis found on file 724.

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

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= 57.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 57

GePol: Total number of spheres = 57

GePol: Number of exposed spheres = 57 (100.00%)

GePol: Number of points = 4682

GePol: Average weight of points = 0.10

GePol: Minimum weight of points = 0.35D-08

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 364

GePol: Fraction of low-weight points (<1% of avg) = 7.77%

GePol: Cavity surface area = 485.766 Ang\*\*2

GePol: Cavity volume = 504.419 Ang\*\*3

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

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PCM non-electrostatic energy = -0.0144354355 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 4373.8046355893 Hartrees.

Leave Link 301 at Sat Jun 15 12:18:20 2019, MaxMem= 1342177280 cpu: 1.2

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 32896 NPrTT= 163506 LenC2= 22875 LenP2D= 61368.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 792 RedAO= T EigKep= 3.44D-05 NBF= 211 187 197 197

NBsUse= 792 1.00D-06 EigRej= -1.00D+00 NBFU= 211 187 197 197

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= 802 802 802 802 802 MxSgAt= 57 MxSgA2= 57.

Leave Link 302 at Sat Jun 15 12:18:22 2019, MaxMem= 1342177280 cpu: 15.6

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

DipDrv: MaxL=1.

Leave Link 303 at Sat Jun 15 12:18:23 2019, MaxMem= 1342177280 cpu: 4.0

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

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

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 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-B1.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7682 S= 0.5090

Leave Link 401 at Sat Jun 15 12:18:29 2019, MaxMem= 1342177280 cpu: 67.7

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 2129573 IEndB= 2129573 NGot= 1342177280 MDV= 1340762408

LenX= 1340762408 LenY= 1340064348

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= 560000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 65763372.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.33D-15 for 758.

Iteration 1 A\*A^-1 deviation from orthogonality is 7.66D-15 for 4442 762.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.66D-15 for 1925.

Iteration 1 A^-1\*A deviation from orthogonality is 1.42D-12 for 2037 2025.

E= -1733.50721191982

DIIS: error= 5.03D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1733.50721191982 IErMin= 1 ErrMin= 5.03D-05

ErrMax= 5.03D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.87D-06 BMatP= 5.87D-06

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

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 0.368 Goal= None Shift= 0.000

Gap= 0.409 Goal= None Shift= 0.000

RMSDP=2.96D-06 MaxDP=7.21D-05 OVMax= 3.01D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.96D-06 CP: 1.00D+00

E= -1733.50721475260 Delta-E= -0.000002832776 Rises=F Damp=F

DIIS: error= 7.41D-06 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1733.50721475260 IErMin= 2 ErrMin= 7.41D-06

ErrMax= 7.41D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.58D-08 BMatP= 5.87D-06

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

Coeff-Com: -0.626D-01 0.106D+01

Coeff: -0.626D-01 0.106D+01

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=4.46D-07 MaxDP=2.31D-05 DE=-2.83D-06 OVMax= 5.43D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 4.05D-07 CP: 1.00D+00 1.06D+00

E= -1733.50721478151 Delta-E= -0.000000028911 Rises=F Damp=F

DIIS: error= 1.13D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1733.50721478151 IErMin= 2 ErrMin= 7.41D-06

ErrMax= 1.13D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.13D-08 BMatP= 9.58D-08

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

Coeff-Com: -0.419D-01 0.566D+00 0.476D+00

Coeff: -0.419D-01 0.566D+00 0.476D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=2.77D-07 MaxDP=1.80D-05 DE=-2.89D-08 OVMax= 3.72D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.86D-07 CP: 1.00D+00 1.07D+00 5.00D-01

E= -1733.50721479724 Delta-E= -0.000000015732 Rises=F Damp=F

DIIS: error= 3.40D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1733.50721479724 IErMin= 4 ErrMin= 3.40D-06

ErrMax= 3.40D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.44D-09 BMatP= 9.13D-08

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

Coeff-Com: -0.988D-02 0.113D+00 0.255D+00 0.642D+00

Coeff: -0.988D-02 0.113D+00 0.255D+00 0.642D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=9.48D-08 MaxDP=5.05D-06 DE=-1.57D-08 OVMax= 1.52D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 6.05D-08 CP: 1.00D+00 1.07D+00 6.24D-01 7.19D-01

E= -1733.50721479940 Delta-E= -0.000000002160 Rises=F Damp=F

DIIS: error= 1.65D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1733.50721479940 IErMin= 5 ErrMin= 1.65D-06

ErrMax= 1.65D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.31D-09 BMatP= 9.44D-09

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

Coeff-Com: -0.161D-02 0.776D-02 0.977D-01 0.364D+00 0.532D+00

Coeff: -0.161D-02 0.776D-02 0.977D-01 0.364D+00 0.532D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=3.65D-08 MaxDP=1.59D-06 DE=-2.16D-09 OVMax= 5.77D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.07D-08 CP: 1.00D+00 1.07D+00 6.20D-01 8.00D-01 5.72D-01

E= -1733.50721479944 Delta-E= -0.000000000043 Rises=F Damp=F

DIIS: error= 4.23D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1733.50721479944 IErMin= 6 ErrMin= 4.23D-07

ErrMax= 4.23D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.48D-10 BMatP= 1.31D-09

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

Coeff-Com: 0.733D-03-0.165D-01 0.111D-01 0.975D-01 0.295D+00 0.613D+00

Coeff: 0.733D-03-0.165D-01 0.111D-01 0.975D-01 0.295D+00 0.613D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=1.16D-08 MaxDP=5.75D-07 DE=-4.27D-11 OVMax= 2.01D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.01D-09 CP: 1.00D+00 1.07D+00 6.26D-01 7.98D-01 6.77D-01

CP: 6.21D-01

E= -1733.50721479990 Delta-E= -0.000000000458 Rises=F Damp=F

DIIS: error= 1.47D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1733.50721479990 IErMin= 7 ErrMin= 1.47D-07

ErrMax= 1.47D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.36D-11 BMatP= 1.48D-10

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

Coeff-Com: 0.506D-03-0.990D-02 0.495D-03 0.341D-01 0.135D+00 0.344D+00

Coeff-Com: 0.496D+00

Coeff: 0.506D-03-0.990D-02 0.495D-03 0.341D-01 0.135D+00 0.344D+00

Coeff: 0.496D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=3.11D-09 MaxDP=1.71D-07 DE=-4.58D-10 OVMax= 5.52D-07

Error on total polarization charges = 0.07593

SCF Done: E(UB3LYP) = -1733.50721480 A.U. after 7 cycles

NFock= 7 Conv=0.31D-08 -V/T= 1.9757

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7682 S= 0.5090

<L.S>= 0.000000000000E+00

KE= 1.776674233683D+03 PE=-1.289475850790D+04 EE= 5.010772423823D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -9.06

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7682, after 0.7503

Leave Link 502 at Sat Jun 15 12:20:15 2019, MaxMem= 1342177280 cpu: 1210.7

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

Compute integral first derivatives.

... and contract with generalized density number 0.

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

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 32896 NPrTT= 163506 LenC2= 22875 LenP2D= 61368.

LDataN: DoStor=T MaxTD1= 6 Len= 172

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

GePol: Maximum number of non-zero 1st derivatives = 197

Leave Link 701 at Sat Jun 15 12:20:25 2019, MaxMem= 1342177280 cpu: 104.7

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

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

Leave Link 702 at Sat Jun 15 12:20:26 2019, MaxMem= 1342177280 cpu: 2.0

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

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=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= 800

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Sat Jun 15 12:20:45 2019, MaxMem= 1342177280 cpu: 226.3

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

Dipole =-4.26325641D-14-6.25277607D-13 8.35411948D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000003114 0.000035324 0.000008549

2 7 -0.000019268 -0.000016483 0.000041697

3 6 0.000027892 0.000008254 -0.000010983

4 6 -0.000006408 -0.000009788 0.000006173

5 6 -0.000009922 -0.000011040 -0.000013595

6 7 0.000000000 0.000026114 0.000001392

7 6 -0.000027892 0.000008254 -0.000010983

8 7 0.000019268 -0.000016483 0.000041697

9 6 -0.000003114 0.000035324 0.000008549

10 6 0.000009922 -0.000011040 -0.000013595

11 6 0.000006408 -0.000009788 0.000006173

12 7 0.000038096 0.000000000 0.000004509

13 6 -0.000009922 0.000011040 -0.000013595

14 6 -0.000006408 0.000009788 0.000006173

15 6 0.000027892 -0.000008254 -0.000010983

16 7 -0.000019268 0.000016483 0.000041697

17 6 0.000003114 -0.000035324 0.000008549

18 7 0.000000000 -0.000026114 0.000001392

19 7 0.000019268 0.000016483 0.000041697

20 6 -0.000027892 -0.000008254 -0.000010983

21 6 0.000006408 0.000009788 0.000006173

22 6 0.000009922 0.000011040 -0.000013595

23 6 -0.000003114 -0.000035324 0.000008549

24 7 -0.000038096 0.000000000 0.000004509

25 30 0.000000000 0.000000000 -0.000140689

26 6 -0.000000346 0.000012560 -0.000003952

27 6 -0.000008718 -0.000003837 0.000000264

28 6 0.000003832 0.000008679 0.000000219

29 6 -0.000011779 -0.000001275 0.000004698

30 6 0.000000346 0.000012560 -0.000003952

31 6 0.000008718 -0.000003837 0.000000264

32 6 -0.000003832 0.000008679 0.000000219

33 6 0.000011779 -0.000001275 0.000004698

34 6 0.000011779 0.000001275 0.000004698

35 6 -0.000003832 -0.000008679 0.000000219

36 6 0.000008718 0.000003837 0.000000264

37 6 0.000000346 -0.000012560 -0.000003952

38 6 -0.000000346 -0.000012560 -0.000003952

39 6 -0.000008718 0.000003837 0.000000264

40 6 0.000003832 -0.000008679 0.000000219

41 6 -0.000011779 0.000001275 0.000004698

42 1 0.000000162 -0.000006182 0.000000423

43 1 0.000005742 0.000000464 -0.000001456

44 1 -0.000000162 -0.000006182 0.000000423

45 1 -0.000005742 0.000000464 -0.000001456

46 1 -0.000005742 -0.000000464 -0.000001456

47 1 -0.000000162 0.000006182 0.000000423

48 1 0.000000162 0.000006182 0.000000423

49 1 0.000005742 -0.000000464 -0.000001456

50 1 0.000000903 -0.000001598 -0.000000722

51 1 0.000001577 -0.000001013 0.000000908

52 1 -0.000000903 -0.000001598 -0.000000722

53 1 -0.000001577 -0.000001013 0.000000908

54 1 -0.000001577 0.000001013 0.000000908

55 1 -0.000000903 0.000001598 -0.000000722

56 1 0.000000903 0.000001598 -0.000000722

57 1 0.000001577 0.000001013 0.000000908

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

Cartesian Forces: Max 0.000140689 RMS 0.000016673

Leave Link 716 at Sat Jun 15 12:20:45 2019, MaxMem= 1342177280 cpu: 1.1

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.000024884 RMS 0.000006881

Search for a local minimum.

Step number 5 out of a maximum of 342

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

RMS Force = .68807D-05 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 4 5

DE= -3.14D-07 DEPred=-2.32D-07 R= 1.35D+00

Trust test= 1.35D+00 RLast= 5.87D-03 DXMaxT set to 3.00D-01

ITU= 0 1 1 1 0

Eigenvalues --- 0.00718 0.01580 0.01586 0.01609 0.01624

Eigenvalues --- 0.01645 0.01658 0.01681 0.01697 0.01761

Eigenvalues --- 0.01772 0.01774 0.01779 0.01780 0.01782

Eigenvalues --- 0.01834 0.01846 0.01853 0.01891 0.01894

Eigenvalues --- 0.01958 0.01959 0.02004 0.02008 0.02008

Eigenvalues --- 0.02008 0.02047 0.02051 0.02051 0.02051

Eigenvalues --- 0.02052 0.02053 0.02053 0.02053 0.02074

Eigenvalues --- 0.02076 0.02105 0.02113 0.02113 0.02113

Eigenvalues --- 0.02119 0.02119 0.02119 0.02122 0.02123

Eigenvalues --- 0.02124 0.02124 0.02124 0.02215 0.02249

Eigenvalues --- 0.02298 0.02323 0.03337 0.03910 0.03928

Eigenvalues --- 0.06819 0.15227 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 0.16030 0.16073 0.16261 0.16367

Eigenvalues --- 0.17687 0.22000 0.22000 0.22000 0.22000

Eigenvalues --- 0.22598 0.22600 0.22600 0.22830 0.24153

Eigenvalues --- 0.24250 0.24511 0.24511 0.24514 0.24530

Eigenvalues --- 0.24629 0.24632 0.24841 0.24848 0.24948

Eigenvalues --- 0.24956 0.24997 0.24997 0.24997 0.24997

Eigenvalues --- 0.26100 0.33728 0.34071 0.34313 0.34482

Eigenvalues --- 0.34804 0.34852 0.35207 0.35218 0.35218

Eigenvalues --- 0.35218 0.35219 0.35243 0.35243 0.35243

Eigenvalues --- 0.35244 0.35245 0.35247 0.35247 0.35247

Eigenvalues --- 0.35252 0.35252 0.35252 0.35377 0.35564

Eigenvalues --- 0.37367 0.37389 0.37565 0.39144 0.40803

Eigenvalues --- 0.40890 0.41918 0.41932 0.41946 0.41959

Eigenvalues --- 0.41973 0.42611 0.43208 0.43248 0.44577

Eigenvalues --- 0.45211 0.45217 0.45287 0.45343 0.45909

Eigenvalues --- 0.45910 0.45911 0.45919 0.46041 0.46122

Eigenvalues --- 0.46178 0.46180 0.46184 0.46709 0.48680

Eigenvalues --- 0.50032 0.50393 0.51371 0.53532 0.53863

Eigenvalues --- 0.55373 0.55380 0.55891 0.58012 0.58039

En-DIIS/RFO-DIIS IScMMF= 0 using points: 5 4 3 2

RFO step: Lambda=-4.99027086D-08.

NNeg= 0 NP= 4 Switch= 2.50D-03 Rises=F DC= 1.78D-05 SmlDif= 1.00D-05

RMS Error= 0.2543290775D-04 NUsed= 4 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.22537 -0.08194 -0.17840 0.03496

Iteration 1 RMS(Cart)= 0.00045052 RMS(Int)= 0.00000007

Iteration 2 RMS(Cart)= 0.00000017 RMS(Int)= 0.00000006

ITry= 1 IFail=0 DXMaxC= 1.95D-03 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.53D-11 for atom 57.

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

(Linear) (Quad) (Total)

R1 2.56175 0.00001 -0.00005 0.00002 -0.00003 2.56172

R2 2.76619 -0.00002 0.00004 -0.00002 0.00001 2.76620

R3 2.53707 0.00002 -0.00005 0.00006 0.00001 2.53708

R4 2.61943 0.00001 0.00001 0.00003 0.00004 2.61948

R5 3.88452 -0.00002 0.00000 -0.00014 -0.00015 3.88437

R6 2.74722 -0.00002 0.00000 -0.00002 -0.00002 2.74720

R7 2.51265 0.00001 -0.00007 0.00004 -0.00003 2.51262

R8 2.68043 0.00000 -0.00004 -0.00001 -0.00005 2.68038

R9 2.64105 -0.00001 -0.00001 0.00001 0.00001 2.64106

R10 2.63515 -0.00001 -0.00002 0.00001 -0.00001 2.63515

R11 2.51265 0.00001 -0.00007 0.00004 -0.00003 2.51262

R12 2.61943 0.00001 0.00001 0.00003 0.00004 2.61948

R13 2.74722 -0.00002 0.00000 -0.00002 -0.00002 2.74720

R14 2.56175 0.00001 -0.00005 0.00002 -0.00003 2.56172

R15 3.88452 -0.00002 0.00000 -0.00014 -0.00015 3.88437

R16 2.76619 -0.00002 0.00004 -0.00002 0.00001 2.76620

R17 2.53707 0.00002 -0.00005 0.00006 0.00001 2.53708

R18 2.68043 0.00000 -0.00004 -0.00001 -0.00005 2.68038

R19 2.63515 -0.00001 -0.00002 0.00001 -0.00001 2.63515

R20 2.64105 -0.00001 -0.00001 0.00001 0.00001 2.64106

R21 2.53707 0.00002 -0.00005 0.00006 0.00001 2.53708

R22 2.68043 0.00000 -0.00004 -0.00001 -0.00005 2.68038

R23 2.76619 -0.00002 0.00004 -0.00002 0.00001 2.76620

R24 2.63515 -0.00001 -0.00002 0.00001 -0.00001 2.63515

R25 2.74722 -0.00002 0.00000 -0.00002 -0.00002 2.74720

R26 2.64105 -0.00001 -0.00001 0.00001 0.00001 2.64106

R27 2.61943 0.00001 0.00001 0.00003 0.00004 2.61948

R28 2.51265 0.00001 -0.00007 0.00004 -0.00003 2.51262

R29 2.56175 0.00001 -0.00005 0.00002 -0.00003 2.56172

R30 3.88452 -0.00002 0.00000 -0.00014 -0.00015 3.88437

R31 2.51265 0.00001 -0.00007 0.00004 -0.00003 2.51262

R32 2.61943 0.00001 0.00001 0.00003 0.00004 2.61948

R33 2.56175 0.00001 -0.00005 0.00002 -0.00003 2.56172

R34 3.88452 -0.00002 0.00000 -0.00014 -0.00015 3.88437

R35 2.74722 -0.00002 0.00000 -0.00002 -0.00002 2.74720

R36 2.68043 0.00000 -0.00004 -0.00001 -0.00005 2.68038

R37 2.64105 -0.00001 -0.00001 0.00001 0.00001 2.64106

R38 2.76619 -0.00002 0.00004 -0.00002 0.00001 2.76620

R39 2.63515 -0.00001 -0.00002 0.00001 -0.00001 2.63515

R40 2.53707 0.00002 -0.00005 0.00006 0.00001 2.53708

R41 2.63084 0.00000 -0.00003 0.00001 -0.00002 2.63082

R42 2.05055 0.00000 0.00001 -0.00001 -0.00001 2.05054

R43 2.66042 -0.00001 0.00001 -0.00002 0.00000 2.66041

R44 2.05023 0.00000 -0.00001 0.00000 0.00000 2.05023

R45 2.62885 0.00000 -0.00003 0.00001 -0.00002 2.62883

R46 2.05080 0.00000 -0.00001 0.00000 0.00000 2.05079

R47 2.05053 0.00000 0.00001 -0.00001 -0.00001 2.05052

R48 2.63084 0.00000 -0.00003 0.00001 -0.00002 2.63082

R49 2.05055 0.00000 0.00001 -0.00001 -0.00001 2.05054

R50 2.66042 -0.00001 0.00001 -0.00002 0.00000 2.66041

R51 2.05023 0.00000 -0.00001 0.00000 0.00000 2.05023

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R55 2.62885 0.00000 -0.00003 0.00001 -0.00002 2.62883

R56 2.05053 0.00000 0.00001 -0.00001 -0.00001 2.05052

R57 2.66042 -0.00001 0.00001 -0.00002 0.00000 2.66041

R58 2.05080 0.00000 -0.00001 0.00000 0.00000 2.05079

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R60 2.05023 0.00000 -0.00001 0.00000 0.00000 2.05023

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R62 2.63084 0.00000 -0.00003 0.00001 -0.00002 2.63082

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R68 2.05053 0.00000 0.00001 -0.00001 -0.00001 2.05052

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A2 2.23752 0.00000 0.00005 -0.00001 0.00004 2.23755

A3 2.15578 -0.00001 -0.00001 -0.00001 -0.00002 2.15576

A4 1.92939 -0.00001 0.00005 -0.00003 0.00002 1.92941

A5 2.17882 0.00000 -0.00001 0.00003 0.00002 2.17885

A6 2.16266 0.00001 0.00003 0.00006 0.00008 2.16275

A7 1.88339 0.00000 -0.00005 0.00001 -0.00004 1.88336

A8 2.22134 0.00000 0.00000 -0.00002 -0.00002 2.22132

A9 2.17832 0.00000 0.00004 0.00001 0.00005 2.17838

A10 1.86069 0.00000 0.00002 0.00001 0.00003 1.86072

A11 2.32143 -0.00001 -0.00003 -0.00001 -0.00004 2.32139

A12 2.10104 0.00000 0.00000 0.00000 0.00001 2.10105

A13 1.86142 0.00000 0.00001 0.00000 0.00001 1.86143

A14 2.31109 -0.00001 -0.00002 0.00000 -0.00002 2.31106

A15 2.11067 0.00000 0.00001 0.00001 0.00002 2.11068

A16 2.20554 -0.00001 0.00004 0.00000 0.00004 2.20558

A17 2.22134 0.00000 0.00000 -0.00002 -0.00002 2.22132

A18 2.17832 0.00000 0.00004 0.00001 0.00005 2.17838

A19 1.88339 0.00000 -0.00005 0.00001 -0.00004 1.88336

A20 1.92939 -0.00001 0.00005 -0.00003 0.00002 1.92941

A21 2.16266 0.00001 0.00003 0.00006 0.00008 2.16275

A22 2.17882 0.00000 -0.00001 0.00003 0.00002 2.17885

A23 1.88984 0.00000 -0.00004 0.00002 -0.00002 1.88982

A24 2.23752 0.00000 0.00005 -0.00001 0.00004 2.23755

A25 2.15578 -0.00001 -0.00001 -0.00001 -0.00002 2.15576

A26 1.86142 0.00000 0.00001 0.00000 0.00001 1.86143

A27 2.31109 -0.00001 -0.00002 0.00000 -0.00002 2.31106

A28 2.11067 0.00000 0.00001 0.00001 0.00002 2.11068

A29 1.86069 0.00000 0.00002 0.00001 0.00003 1.86072

A30 2.32143 -0.00001 -0.00003 -0.00001 -0.00004 2.32139

A31 2.10104 0.00000 0.00000 0.00000 0.00001 2.10105

A32 2.16165 -0.00002 -0.00001 -0.00001 -0.00002 2.16163

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A35 2.31109 -0.00001 -0.00002 0.00000 -0.00002 2.31106

A36 1.86069 0.00000 0.00002 0.00001 0.00003 1.86072

A37 2.10104 0.00000 0.00000 0.00000 0.00001 2.10105

A38 2.32143 -0.00001 -0.00003 -0.00001 -0.00004 2.32139

A39 1.88339 0.00000 -0.00005 0.00001 -0.00004 1.88336

A40 2.17832 0.00000 0.00004 0.00001 0.00005 2.17838

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A42 1.92939 -0.00001 0.00005 -0.00003 0.00002 1.92941

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A45 2.15578 -0.00001 -0.00001 -0.00001 -0.00002 2.15576

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A48 2.20554 -0.00001 0.00004 0.00000 0.00004 2.20558

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A51 2.17882 0.00000 -0.00001 0.00003 0.00002 2.17885

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A53 2.17832 0.00000 0.00004 0.00001 0.00005 2.17838

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A57 2.10104 0.00000 0.00000 0.00000 0.00001 2.10105

A58 1.86142 0.00000 0.00001 0.00000 0.00001 1.86143

A59 2.11067 0.00000 0.00001 0.00001 0.00002 2.11068

A60 2.31109 -0.00001 -0.00002 0.00000 -0.00002 2.31106

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A66 1.52934 0.00001 0.00004 0.00008 0.00012 1.52946

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A71 2.06517 -0.00001 -0.00001 -0.00001 -0.00002 2.06515

A72 2.10628 0.00001 -0.00001 0.00003 0.00002 2.10630

A73 2.11174 0.00000 0.00002 -0.00002 0.00000 2.11174

A74 2.10859 0.00000 0.00000 0.00000 0.00000 2.10859

A75 2.09107 0.00000 0.00000 0.00001 0.00000 2.09107

A76 2.08353 0.00000 0.00000 -0.00001 -0.00001 2.08352

A77 2.11570 0.00000 0.00000 0.00001 0.00001 2.11570

A78 2.08064 0.00000 0.00000 -0.00001 -0.00001 2.08064

A79 2.08684 0.00000 0.00000 0.00001 0.00000 2.08684

A80 2.06519 -0.00001 -0.00001 -0.00001 -0.00002 2.06518

A81 2.10776 0.00001 -0.00001 0.00003 0.00002 2.10777

A82 2.11023 0.00000 0.00002 -0.00002 0.00000 2.11023

A83 2.06517 -0.00001 -0.00001 -0.00001 -0.00002 2.06515

A84 2.10628 0.00001 -0.00001 0.00003 0.00002 2.10630

A85 2.11174 0.00000 0.00002 -0.00002 0.00000 2.11174

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A88 2.08353 0.00000 0.00000 -0.00001 -0.00001 2.08352

A89 2.11570 0.00000 0.00000 0.00001 0.00001 2.11570

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A91 2.08684 0.00000 0.00000 0.00001 0.00000 2.08684

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A103 2.09107 0.00000 0.00000 0.00001 0.00000 2.09107

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A105 2.10628 0.00001 -0.00001 0.00003 0.00002 2.10630

A106 2.11174 0.00000 0.00002 -0.00002 0.00000 2.11174

A107 2.06517 -0.00001 -0.00001 -0.00001 -0.00002 2.06515

A108 2.10628 0.00001 -0.00001 0.00003 0.00002 2.10630

A109 2.11174 0.00000 0.00002 -0.00002 0.00000 2.11174

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A112 2.08353 0.00000 0.00000 -0.00001 -0.00001 2.08352

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A116 2.06519 -0.00001 -0.00001 -0.00001 -0.00002 2.06518

A117 2.10776 0.00001 -0.00001 0.00003 0.00002 2.10777

A118 2.11023 0.00000 0.00002 -0.00002 0.00000 2.11023

D1 0.00915 -0.00001 0.00012 -0.00011 0.00001 0.00917

D2 -2.96956 -0.00001 -0.00036 -0.00046 -0.00082 -2.97038

D3 -3.12129 0.00000 0.00010 0.00006 0.00017 -3.12113

D4 0.18318 -0.00001 -0.00038 -0.00029 -0.00067 0.18251

D5 -0.00512 0.00001 -0.00009 0.00019 0.00010 -0.00502

D6 -3.14118 0.00000 -0.00003 0.00011 0.00008 -3.14111

D7 3.12597 0.00000 -0.00006 0.00002 -0.00004 3.12592

D8 -0.01010 0.00000 -0.00001 -0.00006 -0.00007 -0.01016

D9 0.02289 0.00000 0.00029 0.00005 0.00034 0.02323

D10 -3.10601 0.00000 0.00026 0.00025 0.00051 -3.10550

D11 -0.00954 0.00000 -0.00011 -0.00001 -0.00012 -0.00966

D12 3.11504 0.00000 -0.00017 0.00000 -0.00017 3.11487

D13 2.97098 0.00001 0.00036 0.00034 0.00070 2.97168

D14 -0.18763 0.00001 0.00031 0.00034 0.00065 -0.18698

D15 -3.05840 -0.00001 0.00021 -0.00007 0.00014 -3.05826

D16 -0.26629 0.00001 0.00034 0.00036 0.00069 -0.26560

D17 -1.66416 0.00000 0.00028 0.00015 0.00042 -1.66374

D18 0.26720 -0.00002 -0.00035 -0.00046 -0.00080 0.26640

D19 3.05930 0.00001 -0.00021 -0.00003 -0.00025 3.05906

D20 1.66144 0.00000 -0.00028 -0.00024 -0.00052 1.66092

D21 0.00599 0.00000 0.00006 0.00013 0.00018 0.00617

D22 3.13968 0.00000 0.00002 0.00003 0.00005 3.13972

D23 -3.11911 0.00000 0.00011 0.00012 0.00023 -3.11888

D24 0.01458 0.00000 0.00007 0.00002 0.00009 0.01467

D25 -0.01176 0.00000 -0.00014 -0.00002 -0.00016 -0.01191

D26 3.11012 0.00001 -0.00020 -0.00001 -0.00021 3.10990

D27 -0.00060 0.00000 0.00002 -0.00019 -0.00017 -0.00077

D28 3.13623 0.00000 -0.00003 -0.00012 -0.00015 3.13608

D29 -3.13549 0.00000 0.00005 -0.00010 -0.00005 -3.13555

D30 0.00134 0.00000 0.00000 -0.00003 -0.00003 0.00131

D31 -3.13792 0.00000 0.00002 0.00012 0.00014 -3.13778

D32 0.00528 0.00000 0.00002 0.00007 0.00009 0.00537

D33 -0.00511 0.00000 -0.00002 0.00001 -0.00001 -0.00512

D34 3.13809 0.00000 -0.00002 -0.00004 -0.00006 3.13803

D35 3.13876 0.00000 -0.00004 0.00013 0.00009 3.13885

D36 -0.00390 0.00000 -0.00003 0.00005 0.00002 -0.00389

D37 0.00335 0.00000 0.00002 0.00004 0.00006 0.00341

D38 -3.13932 0.00000 0.00003 -0.00003 -0.00001 -3.13933

D39 0.01176 0.00000 0.00014 0.00002 0.00016 0.01191

D40 -3.11012 -0.00001 0.00020 0.00001 0.00021 -3.10990

D41 -3.11504 0.00000 0.00017 0.00000 0.00017 -3.11487

D42 0.18763 -0.00001 -0.00031 -0.00034 -0.00065 0.18698

D43 0.00954 0.00000 0.00011 0.00001 0.00012 0.00966

D44 -2.97098 -0.00001 -0.00036 -0.00034 -0.00070 -2.97168

D45 3.11911 0.00000 -0.00011 -0.00012 -0.00023 3.11888

D46 -0.01458 0.00000 -0.00007 -0.00002 -0.00009 -0.01467

D47 -0.00599 0.00000 -0.00006 -0.00013 -0.00018 -0.00617

D48 -3.13968 0.00000 -0.00002 -0.00003 -0.00005 -3.13972

D49 -0.00915 0.00001 -0.00012 0.00011 -0.00001 -0.00917

D50 3.12129 0.00000 -0.00010 -0.00006 -0.00017 3.12113

D51 2.96956 0.00001 0.00036 0.00046 0.00082 2.97038

D52 -0.18318 0.00001 0.00038 0.00029 0.00067 -0.18251

D53 -0.26720 0.00002 0.00035 0.00046 0.00080 -0.26640

D54 -1.66144 0.00000 0.00028 0.00024 0.00052 -1.66092

D55 -3.05930 -0.00001 0.00021 0.00003 0.00025 -3.05906

D56 3.05840 0.00001 -0.00021 0.00007 -0.00014 3.05826

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D58 0.26629 -0.00001 -0.00034 -0.00036 -0.00069 0.26560

D59 0.00512 -0.00001 0.00009 -0.00019 -0.00010 0.00502

D60 3.14118 0.00000 0.00003 -0.00011 -0.00008 3.14111

D61 -3.12597 0.00000 0.00006 -0.00002 0.00004 -3.12592

D62 0.01010 0.00000 0.00001 0.00006 0.00007 0.01016

D63 -0.02289 0.00000 -0.00029 -0.00005 -0.00034 -0.02323

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D65 0.00060 0.00000 -0.00002 0.00019 0.00017 0.00077

D66 3.13549 0.00000 -0.00005 0.00010 0.00005 3.13555

D67 -3.13623 0.00000 0.00003 0.00012 0.00015 -3.13608

D68 -0.00134 0.00000 0.00000 0.00003 0.00003 -0.00131

D69 -3.13876 0.00000 0.00004 -0.00013 -0.00009 -3.13885

D70 0.00390 0.00000 0.00003 -0.00005 -0.00002 0.00389

D71 -0.00335 0.00000 -0.00002 -0.00004 -0.00006 -0.00341

D72 3.13932 0.00000 -0.00003 0.00003 0.00001 3.13933

D73 3.13792 0.00000 -0.00002 -0.00012 -0.00014 3.13778

D74 -0.00528 0.00000 -0.00002 -0.00007 -0.00009 -0.00537

D75 0.00511 0.00000 0.00002 -0.00001 0.00001 0.00512

D76 -3.13809 0.00000 0.00002 0.00004 0.00006 -3.13803

D77 3.10601 0.00000 -0.00026 -0.00025 -0.00051 3.10550

D78 -0.02289 0.00000 -0.00029 -0.00005 -0.00034 -0.02323

D79 0.00060 0.00000 -0.00002 0.00019 0.00017 0.00077

D80 3.13549 0.00000 -0.00005 0.00010 0.00005 3.13555

D81 -3.13623 0.00000 0.00003 0.00012 0.00015 -3.13608

D82 -0.00134 0.00000 0.00000 0.00003 0.00003 -0.00131

D83 -3.12597 0.00000 0.00006 -0.00002 0.00004 -3.12592

D84 0.00512 -0.00001 0.00009 -0.00019 -0.00010 0.00502

D85 0.01010 0.00000 0.00001 0.00006 0.00007 0.01016

D86 3.14118 0.00000 0.00003 -0.00011 -0.00008 3.14111

D87 -0.00335 0.00000 -0.00002 -0.00004 -0.00006 -0.00341

D88 3.13932 0.00000 -0.00003 0.00003 0.00001 3.13933

D89 -3.13876 0.00000 0.00004 -0.00013 -0.00009 -3.13885

D90 0.00390 0.00000 0.00003 -0.00005 -0.00002 0.00389

D91 -0.00599 0.00000 -0.00006 -0.00013 -0.00018 -0.00617

D92 3.11911 0.00000 -0.00011 -0.00012 -0.00023 3.11888

D93 -3.13968 0.00000 -0.00002 -0.00003 -0.00005 -3.13972

D94 -0.01458 0.00000 -0.00007 -0.00002 -0.00009 -0.01467

D95 0.00511 0.00000 0.00002 -0.00001 0.00001 0.00512

D96 -3.13809 0.00000 0.00002 0.00004 0.00006 -3.13803

D97 3.13792 0.00000 -0.00002 -0.00012 -0.00014 3.13778

D98 -0.00528 0.00000 -0.00002 -0.00007 -0.00009 -0.00537

D99 0.00954 0.00000 0.00011 0.00001 0.00012 0.00966

D100 -2.97098 -0.00001 -0.00036 -0.00034 -0.00070 -2.97168

D101 -3.11504 0.00000 0.00017 0.00000 0.00017 -3.11487

D102 0.18763 -0.00001 -0.00031 -0.00034 -0.00065 0.18698

D103 -3.11012 -0.00001 0.00020 0.00001 0.00021 -3.10990

D104 0.01176 0.00000 0.00014 0.00002 0.00016 0.01191

D105 3.12129 0.00000 -0.00010 -0.00006 -0.00017 3.12113

D106 -0.00915 0.00001 -0.00012 0.00011 -0.00001 -0.00917

D107 -0.18318 0.00001 0.00038 0.00029 0.00067 -0.18251

D108 2.96956 0.00001 0.00036 0.00046 0.00082 2.97038

D109 -3.05930 -0.00001 0.00021 0.00003 0.00025 -3.05906

D110 -1.66144 0.00000 0.00028 0.00024 0.00052 -1.66092

D111 -0.26720 0.00002 0.00035 0.00046 0.00080 -0.26640

D112 0.26629 -0.00001 -0.00034 -0.00036 -0.00069 0.26560

D113 1.66416 0.00000 -0.00028 -0.00015 -0.00042 1.66374

D114 3.05840 0.00001 -0.00021 0.00007 -0.00014 3.05826

D115 -0.01176 0.00000 -0.00014 -0.00002 -0.00016 -0.01191

D116 3.11012 0.00001 -0.00020 -0.00001 -0.00021 3.10990

D117 3.11504 0.00000 -0.00017 0.00000 -0.00017 3.11487

D118 -0.00954 0.00000 -0.00011 -0.00001 -0.00012 -0.00966

D119 -0.18763 0.00001 0.00031 0.00034 0.00065 -0.18698

D120 2.97098 0.00001 0.00036 0.00034 0.00070 2.97168

D121 0.00915 -0.00001 0.00012 -0.00011 0.00001 0.00917

D122 -3.12129 0.00000 0.00010 0.00006 0.00017 -3.12113

D123 -2.96956 -0.00001 -0.00036 -0.00046 -0.00082 -2.97038

D124 0.18318 -0.00001 -0.00038 -0.00029 -0.00067 0.18251

D125 1.66144 0.00000 -0.00028 -0.00024 -0.00052 1.66092

D126 3.05930 0.00001 -0.00021 -0.00003 -0.00025 3.05906

D127 0.26720 -0.00002 -0.00035 -0.00046 -0.00080 0.26640

D128 -1.66416 0.00000 0.00028 0.00015 0.00042 -1.66374

D129 -0.26629 0.00001 0.00034 0.00036 0.00069 -0.26560

D130 -3.05840 -0.00001 0.00021 -0.00007 0.00014 -3.05826

D131 -3.11911 0.00000 0.00011 0.00012 0.00023 -3.11888

D132 0.01458 0.00000 0.00007 0.00002 0.00009 0.01467

D133 0.00599 0.00000 0.00006 0.00013 0.00018 0.00617

D134 3.13968 0.00000 0.00002 0.00003 0.00005 3.13972

D135 -0.00060 0.00000 0.00002 -0.00019 -0.00017 -0.00077

D136 3.13623 0.00000 -0.00003 -0.00012 -0.00015 3.13608

D137 -3.13549 0.00000 0.00005 -0.00010 -0.00005 -3.13555

D138 0.00134 0.00000 0.00000 -0.00003 -0.00003 0.00131

D139 -3.13792 0.00000 0.00002 0.00012 0.00014 -3.13778

D140 0.00528 0.00000 0.00002 0.00007 0.00009 0.00537

D141 -0.00511 0.00000 -0.00002 0.00001 -0.00001 -0.00512

D142 3.13809 0.00000 -0.00002 -0.00004 -0.00006 3.13803

D143 -0.00512 0.00001 -0.00009 0.00019 0.00010 -0.00502

D144 3.12597 0.00000 -0.00006 0.00002 -0.00004 3.12592

D145 -3.14118 0.00000 -0.00003 0.00011 0.00008 -3.14111

D146 -0.01010 0.00000 -0.00001 -0.00006 -0.00007 -0.01016

D147 0.00335 0.00000 0.00002 0.00004 0.00006 0.00341

D148 -3.13932 0.00000 0.00003 -0.00003 -0.00001 -3.13933

D149 3.13876 0.00000 -0.00004 0.00013 0.00009 3.13885

D150 -0.00390 0.00000 -0.00003 0.00005 0.00002 -0.00389

D151 0.02289 0.00000 0.00029 0.00005 0.00034 0.02323

D152 -3.10601 0.00000 0.00026 0.00025 0.00051 -3.10550

D153 0.00422 0.00000 0.00002 0.00003 0.00004 0.00426

D154 -3.13852 0.00000 0.00001 0.00005 0.00006 -3.13846

D155 -3.13845 0.00000 0.00003 -0.00005 -0.00002 -3.13848

D156 0.00200 0.00000 0.00002 -0.00003 -0.00001 0.00198

D157 -0.00041 0.00000 0.00000 0.00000 0.00000 -0.00042

D158 3.14054 0.00000 -0.00001 -0.00002 -0.00003 3.14052

D159 -3.14087 0.00000 0.00001 -0.00003 -0.00001 -3.14088

D160 0.00009 0.00000 0.00000 -0.00004 -0.00004 0.00005

D161 -0.00427 0.00000 -0.00002 -0.00001 -0.00003 -0.00430

D162 3.13893 0.00000 -0.00002 -0.00006 -0.00008 3.13885

D163 3.13796 0.00000 -0.00001 0.00001 0.00000 3.13796

D164 -0.00203 0.00000 -0.00001 -0.00004 -0.00005 -0.00208

D165 -0.00422 0.00000 -0.00002 -0.00003 -0.00004 -0.00426

D166 3.13852 0.00000 -0.00001 -0.00005 -0.00006 3.13846

D167 3.13845 0.00000 -0.00003 0.00005 0.00002 3.13848

D168 -0.00200 0.00000 -0.00002 0.00003 0.00001 -0.00198

D169 0.00041 0.00000 0.00000 0.00000 0.00000 0.00042

D170 -3.14054 0.00000 0.00001 0.00002 0.00003 -3.14052

D171 3.14087 0.00000 -0.00001 0.00003 0.00001 3.14088

D172 -0.00009 0.00000 0.00000 0.00004 0.00004 -0.00005

D173 0.00427 0.00000 0.00002 0.00001 0.00003 0.00430

D174 -3.13893 0.00000 0.00002 0.00006 0.00008 -3.13885

D175 -3.13796 0.00000 0.00001 -0.00001 0.00000 -3.13796

D176 0.00203 0.00000 0.00001 0.00004 0.00005 0.00208

D177 -0.00427 0.00000 -0.00002 -0.00001 -0.00003 -0.00430

D178 3.13796 0.00000 -0.00001 0.00001 0.00000 3.13796

D179 3.13893 0.00000 -0.00002 -0.00006 -0.00008 3.13885

D180 -0.00203 0.00000 -0.00001 -0.00004 -0.00005 -0.00208

D181 -0.00041 0.00000 0.00000 0.00000 0.00000 -0.00042

D182 -3.14087 0.00000 0.00001 -0.00003 -0.00001 -3.14088

D183 3.14054 0.00000 -0.00001 -0.00002 -0.00003 3.14052

D184 0.00009 0.00000 0.00000 -0.00004 -0.00004 0.00005

D185 0.00422 0.00000 0.00002 0.00003 0.00004 0.00426

D186 -3.13845 0.00000 0.00003 -0.00005 -0.00002 -3.13848

D187 -3.13852 0.00000 0.00001 0.00005 0.00006 -3.13846

D188 0.00200 0.00000 0.00002 -0.00003 -0.00001 0.00198

D189 -0.00422 0.00000 -0.00002 -0.00003 -0.00004 -0.00426

D190 3.13852 0.00000 -0.00001 -0.00005 -0.00006 3.13846

D191 3.13845 0.00000 -0.00003 0.00005 0.00002 3.13848

D192 -0.00200 0.00000 -0.00002 0.00003 0.00001 -0.00198

D193 0.00041 0.00000 0.00000 0.00000 0.00000 0.00042

D194 -3.14054 0.00000 0.00001 0.00002 0.00003 -3.14052

D195 3.14087 0.00000 -0.00001 0.00003 0.00001 3.14088

D196 -0.00009 0.00000 0.00000 0.00004 0.00004 -0.00005

D197 0.00427 0.00000 0.00002 0.00001 0.00003 0.00430

D198 -3.13893 0.00000 0.00002 0.00006 0.00008 -3.13885

D199 -3.13796 0.00000 0.00001 -0.00001 0.00000 -3.13796

D200 0.00203 0.00000 0.00001 0.00004 0.00005 0.00208

Item Value Threshold Converged?

Maximum Force 0.000025 0.000450 YES

RMS Force 0.000007 0.000300 YES

Maximum Displacement 0.001953 0.001800 NO

RMS Displacement 0.000451 0.001200 YES

Predicted change in Energy=-1.233623D-07

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jun 15 12:20:48 2019, MaxMem= 1342177280 cpu: 20.6

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

Stoichiometry C32H16N8Zn(1-,2)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C32H16N4)]

Deg. of freedom 43

Full point group C2V NOp 4

RotChk: IX=0 Diff= 1.64D-16

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 2.772273 1.184599 0.011272

2 7 0 1.438273 1.423126 0.046118

3 6 0 1.186644 2.785828 0.011707

4 6 0 2.465490 3.475468 -0.036881

5 6 0 3.467672 2.471738 -0.038040

6 7 0 0.000000 3.385559 0.002346

7 6 0 -1.186644 2.785828 0.011707

8 7 0 -1.438273 1.423126 0.046118

9 6 0 -2.772273 1.184599 0.011272

10 6 0 -3.467672 2.471738 -0.038040

11 6 0 -2.465490 3.475468 -0.036881

12 7 0 3.404078 0.000000 0.006486

13 6 0 3.467672 -2.471738 -0.038040

14 6 0 2.465490 -3.475468 -0.036881

15 6 0 1.186644 -2.785828 0.011707

16 7 0 1.438273 -1.423126 0.046118

17 6 0 2.772273 -1.184599 0.011272

18 7 0 0.000000 -3.385559 0.002346

19 7 0 -1.438273 -1.423126 0.046118

20 6 0 -1.186644 -2.785828 0.011707

21 6 0 -2.465490 -3.475468 -0.036881

22 6 0 -3.467672 -2.471738 -0.038040

23 6 0 -2.772273 -1.184599 0.011272

24 7 0 -3.404078 0.000000 0.006486

25 30 0 0.000000 0.000000 0.408403

26 6 0 4.819867 -2.808971 -0.086640

27 6 0 5.163187 -4.157451 -0.129918

28 6 0 4.169683 -5.154917 -0.129873

29 6 0 2.818508 -4.826834 -0.086274

30 6 0 -4.819867 -2.808971 -0.086640

31 6 0 -5.163187 -4.157451 -0.129918

32 6 0 -4.169683 -5.154917 -0.129873

33 6 0 -2.818508 -4.826834 -0.086274

34 6 0 -2.818508 4.826834 -0.086274

35 6 0 -4.169683 5.154917 -0.129873

36 6 0 -5.163187 4.157451 -0.129918

37 6 0 -4.819867 2.808971 -0.086640

38 6 0 4.819867 2.808971 -0.086640

39 6 0 5.163187 4.157451 -0.129918

40 6 0 4.169683 5.154917 -0.129873

41 6 0 2.818508 4.826834 -0.086274

42 1 0 5.583123 -2.037692 -0.089448

43 1 0 2.056911 -5.599739 -0.089010

44 1 0 -5.583123 -2.037692 -0.089448

45 1 0 -2.056911 -5.599739 -0.089010

46 1 0 -2.056911 5.599739 -0.089010

47 1 0 -5.583123 2.037692 -0.089448

48 1 0 5.583123 2.037692 -0.089448

49 1 0 2.056911 5.599739 -0.089010

50 1 0 -4.466568 6.198153 -0.165178

51 1 0 -6.208147 4.447087 -0.165237

52 1 0 4.466568 6.198153 -0.165178

53 1 0 6.208147 4.447087 -0.165237

54 1 0 6.208147 -4.447087 -0.165237

55 1 0 4.466568 -6.198153 -0.165178

56 1 0 -4.466568 -6.198153 -0.165178

57 1 0 -6.208147 -4.447087 -0.165237

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

Rotational constants (GHZ): 0.0880319 0.0879157 0.0440907

Leave Link 202 at Sat Jun 15 12:20:48 2019, MaxMem= 1342177280 cpu: 0.0

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 225 symmetry adapted cartesian basis functions of A1 symmetry.

There are 196 symmetry adapted cartesian basis functions of A2 symmetry.

There are 207 symmetry adapted cartesian basis functions of B1 symmetry.

There are 207 symmetry adapted cartesian basis functions of B2 symmetry.

There are 211 symmetry adapted basis functions of A1 symmetry.

There are 187 symmetry adapted basis functions of A2 symmetry.

There are 197 symmetry adapted basis functions of B1 symmetry.

There are 197 symmetry adapted basis functions of B2 symmetry.

792 basis functions, 1399 primitive gaussians, 835 cartesian basis functions

139 alpha electrons 138 beta electrons

nuclear repulsion energy 4373.9994456777 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= 57 NActive= 57 NUniq= 16 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1642466346 Hartrees.

Nuclear repulsion after empirical dispersion term = 4373.8351990431 Hartrees.

No density basis found on file 724.

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

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= 57.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 57

GePol: Total number of spheres = 57

GePol: Number of exposed spheres = 57 (100.00%)

GePol: Number of points = 4682

GePol: Average weight of points = 0.10

GePol: Minimum weight of points = 0.58D-08

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 364

GePol: Fraction of low-weight points (<1% of avg) = 7.77%

GePol: Cavity surface area = 485.786 Ang\*\*2

GePol: Cavity volume = 504.432 Ang\*\*3

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

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PCM non-electrostatic energy = -0.0144338412 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 4373.8207652019 Hartrees.

Leave Link 301 at Sat Jun 15 12:20:48 2019, MaxMem= 1342177280 cpu: 2.3

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 32896 NPrTT= 163506 LenC2= 22875 LenP2D= 61368.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 792 RedAO= T EigKep= 3.44D-05 NBF= 211 187 197 197

NBsUse= 792 1.00D-06 EigRej= -1.00D+00 NBFU= 211 187 197 197

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= 802 802 802 802 802 MxSgAt= 57 MxSgA2= 57.

Leave Link 302 at Sat Jun 15 12:20:50 2019, MaxMem= 1342177280 cpu: 18.0

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

DipDrv: MaxL=1.

Leave Link 303 at Sat Jun 15 12:20:50 2019, MaxMem= 1342177280 cpu: 2.5

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

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

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 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 (B2) (A1) (A2) (B1) (B2) (A1) (B1) (A1) (B1) (A2)

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The electronic state of the initial guess is 2-B1.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7682 S= 0.5090

Leave Link 401 at Sat Jun 15 12:20:56 2019, MaxMem= 1342177280 cpu: 63.9

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 2129573 IEndB= 2129573 NGot= 1342177280 MDV= 1340762408

LenX= 1340762408 LenY= 1340064348

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= 560000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 65763372.

Iteration 1 A\*A^-1 deviation from unit magnitude is 9.55D-15 for 4681.

Iteration 1 A\*A^-1 deviation from orthogonality is 6.41D-15 for 4614 761.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.77D-15 for 4681.

Iteration 1 A^-1\*A deviation from orthogonality is 1.53D-12 for 3873 3831.

E= -1733.50721358826

DIIS: error= 3.62D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1733.50721358826 IErMin= 1 ErrMin= 3.62D-05

ErrMax= 3.62D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.80D-06 BMatP= 2.80D-06

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

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 0.368 Goal= None Shift= 0.000

Gap= 0.409 Goal= None Shift= 0.000

RMSDP=2.18D-06 MaxDP=5.19D-05 OVMax= 1.81D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.18D-06 CP: 1.00D+00

E= -1733.50721491967 Delta-E= -0.000001331409 Rises=F Damp=F

DIIS: error= 1.02D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1733.50721491967 IErMin= 2 ErrMin= 1.02D-05

ErrMax= 1.02D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.77D-08 BMatP= 2.80D-06

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

Coeff-Com: -0.559D-01 0.106D+01

Coeff: -0.559D-01 0.106D+01

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=2.99D-07 MaxDP=8.56D-06 DE=-1.33D-06 OVMax= 3.51D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.77D-07 CP: 1.00D+00 1.05D+00

E= -1733.50721493228 Delta-E= -0.000000012602 Rises=F Damp=F

DIIS: error= 1.55D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1733.50721493228 IErMin= 2 ErrMin= 1.02D-05

ErrMax= 1.55D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.94D-08 BMatP= 4.77D-08

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

Coeff-Com: -0.421D-01 0.595D+00 0.447D+00

Coeff: -0.421D-01 0.595D+00 0.447D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=1.70D-07 MaxDP=7.66D-06 DE=-1.26D-08 OVMax= 2.68D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.14D-07 CP: 1.00D+00 1.06D+00 5.48D-01

E= -1733.50721494105 Delta-E= -0.000000008776 Rises=F Damp=F

DIIS: error= 1.38D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1733.50721494105 IErMin= 4 ErrMin= 1.38D-06

ErrMax= 1.38D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.00D-09 BMatP= 4.77D-08

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

Coeff-Com: -0.126D-01 0.151D+00 0.223D+00 0.639D+00

Coeff: -0.126D-01 0.151D+00 0.223D+00 0.639D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=6.11D-08 MaxDP=2.48D-06 DE=-8.78D-09 OVMax= 1.21D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.50D-08 CP: 1.00D+00 1.06D+00 6.51D-01 7.38D-01

E= -1733.50721494174 Delta-E= -0.000000000689 Rises=F Damp=F

DIIS: error= 1.88D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1733.50721494174 IErMin= 4 ErrMin= 1.38D-06

ErrMax= 1.88D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.19D-09 BMatP= 4.00D-09

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

Coeff-Com: -0.146D-02 0.191D-02 0.713D-01 0.409D+00 0.519D+00

Coeff: -0.146D-02 0.191D-02 0.713D-01 0.409D+00 0.519D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=2.78D-08 MaxDP=1.26D-06 DE=-6.89D-10 OVMax= 5.40D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.27D-08 CP: 1.00D+00 1.06D+00 6.36D-01 8.55D-01 5.53D-01

E= -1733.50721494218 Delta-E= -0.000000000442 Rises=F Damp=F

DIIS: error= 2.35D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1733.50721494218 IErMin= 6 ErrMin= 2.35D-07

ErrMax= 2.35D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.05D-11 BMatP= 1.19D-09

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

Coeff-Com: 0.674D-03-0.163D-01 0.577D-02 0.102D+00 0.222D+00 0.686D+00

Coeff: 0.674D-03-0.163D-01 0.577D-02 0.102D+00 0.222D+00 0.686D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=6.25D-09 MaxDP=2.96D-07 DE=-4.42D-10 OVMax= 9.00D-07

Error on total polarization charges = 0.07593

SCF Done: E(UB3LYP) = -1733.50721494 A.U. after 6 cycles

NFock= 6 Conv=0.63D-08 -V/T= 1.9757

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7682 S= 0.5090

<L.S>= 0.000000000000E+00

KE= 1.776674872624D+03 PE=-1.289479186592D+04 EE= 5.010789013152D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -9.06

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7682, after 0.7503

Leave Link 502 at Sat Jun 15 12:22:32 2019, MaxMem= 1342177280 cpu: 1086.2

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

Compute integral first derivatives.

... and contract with generalized density number 0.

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

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 32896 NPrTT= 163506 LenC2= 22875 LenP2D= 61368.

LDataN: DoStor=T MaxTD1= 6 Len= 172

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

GePol: Maximum number of non-zero 1st derivatives = 197

Leave Link 701 at Sat Jun 15 12:22:41 2019, MaxMem= 1342177280 cpu: 102.3

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

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

Leave Link 702 at Sat Jun 15 12:22:42 2019, MaxMem= 1342177280 cpu: 1.7

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

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=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= 800

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Sat Jun 15 12:23:00 2019, MaxMem= 1342177280 cpu: 216.7

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

Dipole =-2.91322522D-13 4.76063633D-13 8.32377638D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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1 6 0.000015654 0.000041237 -0.000001665

2 7 -0.000026880 -0.000008736 0.000020867

3 6 0.000034796 -0.000018413 0.000003755

4 6 -0.000017834 0.000011744 -0.000003122

5 6 -0.000001962 -0.000028252 0.000005566

6 7 0.000000000 0.000041476 -0.000003507

7 6 -0.000034796 -0.000018413 0.000003755

8 7 0.000026880 -0.000008736 0.000020867

9 6 -0.000015654 0.000041237 -0.000001665

10 6 0.000001962 -0.000028252 0.000005566

11 6 0.000017834 0.000011744 -0.000003122

12 7 0.000027199 0.000000000 -0.000007478

13 6 -0.000001962 0.000028252 0.000005566

14 6 -0.000017834 -0.000011744 -0.000003122

15 6 0.000034796 0.000018413 0.000003755

16 7 -0.000026880 0.000008736 0.000020867

17 6 0.000015654 -0.000041237 -0.000001665

18 7 0.000000000 -0.000041476 -0.000003507

19 7 0.000026880 0.000008736 0.000020867

20 6 -0.000034796 0.000018413 0.000003755

21 6 0.000017834 -0.000011744 -0.000003122

22 6 0.000001962 0.000028252 0.000005566

23 6 -0.000015654 -0.000041237 -0.000001665

24 7 -0.000027199 0.000000000 -0.000007478

25 30 0.000000000 0.000000000 -0.000089598

26 6 -0.000000095 0.000009757 0.000003641

27 6 -0.000005036 -0.000007769 -0.000000392

28 6 0.000009093 0.000004251 -0.000000035

29 6 -0.000011632 0.000003048 0.000000215

30 6 0.000000095 0.000009757 0.000003641

31 6 0.000005036 -0.000007769 -0.000000392

32 6 -0.000009093 0.000004251 -0.000000035

33 6 0.000011632 0.000003048 0.000000215

34 6 0.000011632 -0.000003048 0.000000215

35 6 -0.000009093 -0.000004251 -0.000000035

36 6 0.000005036 0.000007769 -0.000000392

37 6 0.000000095 -0.000009757 0.000003641

38 6 -0.000000095 -0.000009757 0.000003641

39 6 -0.000005036 0.000007769 -0.000000392

40 6 0.000009093 -0.000004251 -0.000000035

41 6 -0.000011632 -0.000003048 0.000000215

42 1 0.000001100 -0.000003862 -0.000000470

43 1 0.000003339 -0.000000678 0.000000165

44 1 -0.000001100 -0.000003862 -0.000000470

45 1 -0.000003339 -0.000000678 0.000000165

46 1 -0.000003339 0.000000678 0.000000165

47 1 -0.000001100 0.000003862 -0.000000470

48 1 0.000001100 0.000003862 -0.000000470

49 1 0.000003339 0.000000678 0.000000165

50 1 0.000000632 0.000000404 0.000000009

51 1 -0.000000348 -0.000000768 -0.000000642

52 1 -0.000000632 0.000000404 0.000000009

53 1 0.000000348 -0.000000768 -0.000000642

54 1 0.000000348 0.000000768 -0.000000642

55 1 -0.000000632 -0.000000404 0.000000009

56 1 0.000000632 -0.000000404 0.000000009

57 1 -0.000000348 0.000000768 -0.000000642

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

Cartesian Forces: Max 0.000089598 RMS 0.000015130

Leave Link 716 at Sat Jun 15 12:23:01 2019, MaxMem= 1342177280 cpu: 3.2

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.000022867 RMS 0.000006321

Search for a local minimum.

Step number 6 out of a maximum of 342

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

RMS Force = .63210D-05 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 4 5

6

DE= -1.42D-07 DEPred=-1.23D-07 R= 1.15D+00

Trust test= 1.15D+00 RLast= 4.33D-03 DXMaxT set to 3.00D-01

ITU= 0 0 1 1 1 0

Eigenvalues --- 0.00617 0.01586 0.01586 0.01609 0.01624

Eigenvalues --- 0.01645 0.01661 0.01681 0.01697 0.01760

Eigenvalues --- 0.01772 0.01774 0.01779 0.01780 0.01782

Eigenvalues --- 0.01834 0.01846 0.01855 0.01891 0.01894

Eigenvalues --- 0.01958 0.01959 0.02005 0.02008 0.02008

Eigenvalues --- 0.02008 0.02049 0.02051 0.02051 0.02051

Eigenvalues --- 0.02052 0.02053 0.02053 0.02053 0.02075

Eigenvalues --- 0.02076 0.02112 0.02113 0.02113 0.02113

Eigenvalues --- 0.02119 0.02119 0.02119 0.02122 0.02124

Eigenvalues --- 0.02124 0.02124 0.02124 0.02249 0.02293

Eigenvalues --- 0.02323 0.02585 0.03337 0.03903 0.03920

Eigenvalues --- 0.05674 0.15228 0.15824 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 0.16040 0.16261 0.16367

Eigenvalues --- 0.16919 0.22000 0.22000 0.22000 0.22001

Eigenvalues --- 0.22598 0.22600 0.22600 0.22631 0.24159

Eigenvalues --- 0.24298 0.24511 0.24511 0.24530 0.24530

Eigenvalues --- 0.24631 0.24635 0.24843 0.24949 0.24956

Eigenvalues --- 0.24995 0.24997 0.24997 0.24997 0.25087

Eigenvalues --- 0.26077 0.33728 0.34071 0.34131 0.34313

Eigenvalues --- 0.34805 0.34851 0.35191 0.35218 0.35218

Eigenvalues --- 0.35218 0.35219 0.35239 0.35243 0.35243

Eigenvalues --- 0.35243 0.35245 0.35247 0.35247 0.35247

Eigenvalues --- 0.35252 0.35252 0.35252 0.35369 0.35752

Eigenvalues --- 0.37367 0.37389 0.37496 0.37565 0.40803

Eigenvalues --- 0.40889 0.41932 0.41946 0.41949 0.41959

Eigenvalues --- 0.41972 0.42766 0.43208 0.43248 0.44577

Eigenvalues --- 0.45211 0.45217 0.45226 0.45343 0.45824

Eigenvalues --- 0.45910 0.45911 0.45919 0.46042 0.46122

Eigenvalues --- 0.46178 0.46180 0.46184 0.46712 0.47614

Eigenvalues --- 0.50019 0.50394 0.51372 0.53534 0.53685

Eigenvalues --- 0.55373 0.55380 0.56574 0.58012 0.58039

En-DIIS/RFO-DIIS IScMMF= 0 using points: 6 5 4 3 2

RFO step: Lambda=-3.64378458D-08.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 1.78D-05 SmlDif= 1.00D-05

RMS Error= 0.1833966907D-04 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.56085 -0.29504 -0.51436 0.27305 -0.02450

Iteration 1 RMS(Cart)= 0.00010724 RMS(Int)= 0.00000005

Iteration 2 RMS(Cart)= 0.00000005 RMS(Int)= 0.00000004

ITry= 1 IFail=0 DXMaxC= 1.50D-03 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 2.43D-11 for atom 57.

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

(Linear) (Quad) (Total)

R1 2.56172 0.00002 0.00001 0.00002 0.00003 2.56175

R2 2.76620 -0.00002 -0.00005 -0.00002 -0.00007 2.76613

R3 2.53708 0.00002 0.00006 0.00000 0.00006 2.53714

R4 2.61948 0.00000 0.00003 0.00000 0.00002 2.61950

R5 3.88437 -0.00001 -0.00019 -0.00003 -0.00022 3.88415

R6 2.74720 -0.00001 -0.00005 0.00000 -0.00005 2.74715

R7 2.51262 0.00002 0.00003 0.00001 0.00005 2.51266

R8 2.68038 0.00001 -0.00004 0.00007 0.00002 2.68040

R9 2.64106 0.00000 -0.00001 0.00001 0.00000 2.64105

R10 2.63515 0.00000 -0.00001 0.00001 0.00000 2.63515

R11 2.51262 0.00002 0.00003 0.00001 0.00005 2.51266

R12 2.61948 0.00000 0.00003 0.00000 0.00002 2.61950

R13 2.74720 -0.00001 -0.00005 0.00000 -0.00005 2.74715

R14 2.56172 0.00002 0.00001 0.00002 0.00003 2.56175

R15 3.88437 -0.00001 -0.00019 -0.00003 -0.00022 3.88415

R16 2.76620 -0.00002 -0.00005 -0.00002 -0.00007 2.76613

R17 2.53708 0.00002 0.00006 0.00000 0.00006 2.53714

R18 2.68038 0.00001 -0.00004 0.00007 0.00002 2.68040

R19 2.63515 0.00000 -0.00001 0.00001 0.00000 2.63515

R20 2.64106 0.00000 -0.00001 0.00001 0.00000 2.64105

R21 2.53708 0.00002 0.00006 0.00000 0.00006 2.53714

R22 2.68038 0.00001 -0.00004 0.00007 0.00002 2.68040

R23 2.76620 -0.00002 -0.00005 -0.00002 -0.00007 2.76613

R24 2.63515 0.00000 -0.00001 0.00001 0.00000 2.63515

R25 2.74720 -0.00001 -0.00005 0.00000 -0.00005 2.74715

R26 2.64106 0.00000 -0.00001 0.00001 0.00000 2.64105

R27 2.61948 0.00000 0.00003 0.00000 0.00002 2.61950

R28 2.51262 0.00002 0.00003 0.00001 0.00005 2.51266

R29 2.56172 0.00002 0.00001 0.00002 0.00003 2.56175

R30 3.88437 -0.00001 -0.00019 -0.00003 -0.00022 3.88415

R31 2.51262 0.00002 0.00003 0.00001 0.00005 2.51266

R32 2.61948 0.00000 0.00003 0.00000 0.00002 2.61950

R33 2.56172 0.00002 0.00001 0.00002 0.00003 2.56175

R34 3.88437 -0.00001 -0.00019 -0.00003 -0.00022 3.88415

R35 2.74720 -0.00001 -0.00005 0.00000 -0.00005 2.74715

R36 2.68038 0.00001 -0.00004 0.00007 0.00002 2.68040

R37 2.64106 0.00000 -0.00001 0.00001 0.00000 2.64105

R38 2.76620 -0.00002 -0.00005 -0.00002 -0.00007 2.76613

R39 2.63515 0.00000 -0.00001 0.00001 0.00000 2.63515

R40 2.53708 0.00002 0.00006 0.00000 0.00006 2.53714

R41 2.63082 0.00000 -0.00001 0.00001 0.00001 2.63083

R42 2.05054 0.00000 -0.00003 0.00002 -0.00001 2.05053

R43 2.66041 -0.00001 -0.00004 0.00003 -0.00001 2.66040

R44 2.05023 0.00000 -0.00001 0.00001 0.00000 2.05023

R45 2.62883 0.00000 -0.00001 0.00001 0.00001 2.62884

R46 2.05079 0.00000 -0.00001 0.00001 0.00000 2.05079

R47 2.05052 0.00000 -0.00003 0.00002 -0.00001 2.05052

R48 2.63082 0.00000 -0.00001 0.00001 0.00001 2.63083

R49 2.05054 0.00000 -0.00003 0.00002 -0.00001 2.05053

R50 2.66041 -0.00001 -0.00004 0.00003 -0.00001 2.66040

R51 2.05023 0.00000 -0.00001 0.00001 0.00000 2.05023

R52 2.62883 0.00000 -0.00001 0.00001 0.00001 2.62884

R53 2.05079 0.00000 -0.00001 0.00001 0.00000 2.05079

R54 2.05052 0.00000 -0.00003 0.00002 -0.00001 2.05052

R55 2.62883 0.00000 -0.00001 0.00001 0.00001 2.62884

R56 2.05052 0.00000 -0.00003 0.00002 -0.00001 2.05052

R57 2.66041 -0.00001 -0.00004 0.00003 -0.00001 2.66040

R58 2.05079 0.00000 -0.00001 0.00001 0.00000 2.05079

R59 2.63082 0.00000 -0.00001 0.00001 0.00001 2.63083

R60 2.05023 0.00000 -0.00001 0.00001 0.00000 2.05023

R61 2.05054 0.00000 -0.00003 0.00002 -0.00001 2.05053

R62 2.63082 0.00000 -0.00001 0.00001 0.00001 2.63083

R63 2.05054 0.00000 -0.00003 0.00002 -0.00001 2.05053

R64 2.66041 -0.00001 -0.00004 0.00003 -0.00001 2.66040

R65 2.05023 0.00000 -0.00001 0.00001 0.00000 2.05023

R66 2.62883 0.00000 -0.00001 0.00001 0.00001 2.62884

R67 2.05079 0.00000 -0.00001 0.00001 0.00000 2.05079

R68 2.05052 0.00000 -0.00003 0.00002 -0.00001 2.05052

A1 1.88982 0.00000 0.00003 -0.00003 0.00000 1.88982

A2 2.23755 0.00000 0.00000 0.00002 0.00001 2.23757

A3 2.15576 0.00000 -0.00002 0.00001 -0.00001 2.15575

A4 1.92941 -0.00001 -0.00005 0.00004 -0.00001 1.92940

A5 2.17885 0.00001 0.00004 -0.00001 0.00003 2.17888

A6 2.16275 0.00000 0.00006 -0.00001 0.00005 2.16279

A7 1.88336 0.00001 0.00002 -0.00002 0.00000 1.88335

A8 2.22132 0.00000 -0.00002 0.00003 0.00001 2.22133

A9 2.17838 -0.00001 0.00000 -0.00001 -0.00001 2.17837

A10 1.86072 0.00000 0.00001 0.00000 0.00001 1.86072

A11 2.32139 0.00000 -0.00002 0.00000 -0.00002 2.32138

A12 2.10105 0.00000 0.00001 0.00000 0.00001 2.10106

A13 1.86143 0.00000 0.00000 0.00001 0.00001 1.86144

A14 2.31106 0.00000 -0.00001 0.00000 -0.00001 2.31105

A15 2.11068 0.00000 0.00001 0.00000 0.00000 2.11068

A16 2.20558 -0.00002 -0.00002 -0.00002 -0.00004 2.20554

A17 2.22132 0.00000 -0.00002 0.00003 0.00001 2.22133

A18 2.17838 -0.00001 0.00000 -0.00001 -0.00001 2.17837

A19 1.88336 0.00001 0.00002 -0.00002 0.00000 1.88335

A20 1.92941 -0.00001 -0.00005 0.00004 -0.00001 1.92940

A21 2.16275 0.00000 0.00006 -0.00001 0.00005 2.16279

A22 2.17885 0.00001 0.00004 -0.00001 0.00003 2.17888

A23 1.88982 0.00000 0.00003 -0.00003 0.00000 1.88982

A24 2.23755 0.00000 0.00000 0.00002 0.00001 2.23757

A25 2.15576 0.00000 -0.00002 0.00001 -0.00001 2.15575

A26 1.86143 0.00000 0.00000 0.00001 0.00001 1.86144

A27 2.31106 0.00000 -0.00001 0.00000 -0.00001 2.31105

A28 2.11068 0.00000 0.00001 0.00000 0.00000 2.11068

A29 1.86072 0.00000 0.00001 0.00000 0.00001 1.86072

A30 2.32139 0.00000 -0.00002 0.00000 -0.00002 2.32138

A31 2.10105 0.00000 0.00001 0.00000 0.00001 2.10106

A32 2.16163 -0.00001 -0.00004 0.00001 -0.00004 2.16159

A33 1.86143 0.00000 0.00000 0.00001 0.00001 1.86144

A34 2.11068 0.00000 0.00001 0.00000 0.00000 2.11068

A35 2.31106 0.00000 -0.00001 0.00000 -0.00001 2.31105

A36 1.86072 0.00000 0.00001 0.00000 0.00001 1.86072

A37 2.10105 0.00000 0.00001 0.00000 0.00001 2.10106

A38 2.32139 0.00000 -0.00002 0.00000 -0.00002 2.32138

A39 1.88336 0.00001 0.00002 -0.00002 0.00000 1.88335

A40 2.17838 -0.00001 0.00000 -0.00001 -0.00001 2.17837

A41 2.22132 0.00000 -0.00002 0.00003 0.00001 2.22133

A42 1.92941 -0.00001 -0.00005 0.00004 -0.00001 1.92940

A43 2.16275 0.00000 0.00006 -0.00001 0.00005 2.16279

A44 2.17885 0.00001 0.00004 -0.00001 0.00003 2.17888

A45 2.15576 0.00000 -0.00002 0.00001 -0.00001 2.15575

A46 2.23755 0.00000 0.00000 0.00002 0.00001 2.23757

A47 1.88982 0.00000 0.00003 -0.00003 0.00000 1.88982

A48 2.20558 -0.00002 -0.00002 -0.00002 -0.00004 2.20554

A49 1.92941 -0.00001 -0.00005 0.00004 -0.00001 1.92940

A50 2.16275 0.00000 0.00006 -0.00001 0.00005 2.16279

A51 2.17885 0.00001 0.00004 -0.00001 0.00003 2.17888

A52 2.22132 0.00000 -0.00002 0.00003 0.00001 2.22133

A53 2.17838 -0.00001 0.00000 -0.00001 -0.00001 2.17837

A54 1.88336 0.00001 0.00002 -0.00002 0.00000 1.88335

A55 1.86072 0.00000 0.00001 0.00000 0.00001 1.86072

A56 2.32139 0.00000 -0.00002 0.00000 -0.00002 2.32138

A57 2.10105 0.00000 0.00001 0.00000 0.00001 2.10106

A58 1.86143 0.00000 0.00000 0.00001 0.00001 1.86144

A59 2.11068 0.00000 0.00001 0.00000 0.00000 2.11068

A60 2.31106 0.00000 -0.00001 0.00000 -0.00001 2.31105

A61 1.88982 0.00000 0.00003 -0.00003 0.00000 1.88982

A62 2.23755 0.00000 0.00000 0.00002 0.00001 2.23757

A63 2.15576 0.00000 -0.00002 0.00001 -0.00001 2.15575

A64 2.16163 -0.00001 -0.00004 0.00001 -0.00004 2.16159

A65 1.54999 0.00000 0.00006 0.00005 0.00012 1.55010

A66 1.52946 0.00000 0.00007 0.00006 0.00013 1.52959

A67 2.78724 0.00002 0.00039 0.00032 0.00070 2.78795

A68 2.78724 0.00002 0.00039 0.00032 0.00070 2.78795

A69 1.52946 0.00000 0.00007 0.00006 0.00013 1.52959

A70 1.54999 0.00000 0.00006 0.00005 0.00012 1.55010

A71 2.06515 0.00000 -0.00002 0.00000 -0.00002 2.06513

A72 2.10630 0.00000 0.00005 0.00000 0.00005 2.10634

A73 2.11174 0.00000 -0.00003 0.00001 -0.00002 2.11171

A74 2.10859 0.00000 0.00001 0.00001 0.00002 2.10861

A75 2.09107 0.00000 0.00000 -0.00002 -0.00001 2.09106

A76 2.08352 0.00000 -0.00001 0.00001 0.00000 2.08352

A77 2.11570 0.00000 0.00001 0.00000 0.00001 2.11572

A78 2.08064 0.00000 -0.00002 0.00001 0.00000 2.08063

A79 2.08684 0.00000 0.00001 -0.00002 -0.00001 2.08683

A80 2.06518 0.00000 -0.00002 0.00000 -0.00002 2.06515

A81 2.10777 0.00000 0.00004 0.00000 0.00004 2.10781

A82 2.11023 0.00000 -0.00002 0.00001 -0.00002 2.11022

A83 2.06515 0.00000 -0.00002 0.00000 -0.00002 2.06513

A84 2.10630 0.00000 0.00005 0.00000 0.00005 2.10634

A85 2.11174 0.00000 -0.00003 0.00001 -0.00002 2.11171

A86 2.10859 0.00000 0.00001 0.00001 0.00002 2.10861

A87 2.09107 0.00000 0.00000 -0.00002 -0.00001 2.09106

A88 2.08352 0.00000 -0.00001 0.00001 0.00000 2.08352

A89 2.11570 0.00000 0.00001 0.00000 0.00001 2.11572

A90 2.08064 0.00000 -0.00002 0.00001 0.00000 2.08063

A91 2.08684 0.00000 0.00001 -0.00002 -0.00001 2.08683

A92 2.06518 0.00000 -0.00002 0.00000 -0.00002 2.06515

A93 2.10777 0.00000 0.00004 0.00000 0.00004 2.10781

A94 2.11023 0.00000 -0.00002 0.00001 -0.00002 2.11022

A95 2.06518 0.00000 -0.00002 0.00000 -0.00002 2.06515

A96 2.10777 0.00000 0.00004 0.00000 0.00004 2.10781

A97 2.11023 0.00000 -0.00002 0.00001 -0.00002 2.11022

A98 2.11570 0.00000 0.00001 0.00000 0.00001 2.11572

A99 2.08684 0.00000 0.00001 -0.00002 -0.00001 2.08683

A100 2.08064 0.00000 -0.00002 0.00001 0.00000 2.08063

A101 2.10859 0.00000 0.00001 0.00001 0.00002 2.10861

A102 2.08352 0.00000 -0.00001 0.00001 0.00000 2.08352

A103 2.09107 0.00000 0.00000 -0.00002 -0.00001 2.09106

A104 2.06515 0.00000 -0.00002 0.00000 -0.00002 2.06513

A105 2.10630 0.00000 0.00005 0.00000 0.00005 2.10634

A106 2.11174 0.00000 -0.00003 0.00001 -0.00002 2.11171

A107 2.06515 0.00000 -0.00002 0.00000 -0.00002 2.06513

A108 2.10630 0.00000 0.00005 0.00000 0.00005 2.10634

A109 2.11174 0.00000 -0.00003 0.00001 -0.00002 2.11171

A110 2.10859 0.00000 0.00001 0.00001 0.00002 2.10861

A111 2.09107 0.00000 0.00000 -0.00002 -0.00001 2.09106

A112 2.08352 0.00000 -0.00001 0.00001 0.00000 2.08352

A113 2.11570 0.00000 0.00001 0.00000 0.00001 2.11572

A114 2.08064 0.00000 -0.00002 0.00001 0.00000 2.08063

A115 2.08684 0.00000 0.00001 -0.00002 -0.00001 2.08683

A116 2.06518 0.00000 -0.00002 0.00000 -0.00002 2.06515

A117 2.10777 0.00000 0.00004 0.00000 0.00004 2.10781

A118 2.11023 0.00000 -0.00002 0.00001 -0.00002 2.11022

D1 0.00917 0.00000 0.00005 0.00002 0.00007 0.00924

D2 -2.97038 0.00000 -0.00029 -0.00008 -0.00037 -2.97075

D3 -3.12113 0.00000 0.00002 -0.00003 -0.00001 -3.12113

D4 0.18251 -0.00001 -0.00032 -0.00012 -0.00045 0.18206

D5 -0.00502 0.00000 -0.00005 -0.00004 -0.00009 -0.00511

D6 -3.14111 0.00000 -0.00002 -0.00004 -0.00006 -3.14117

D7 3.12592 0.00000 -0.00002 0.00000 -0.00001 3.12591

D8 -0.01016 0.00000 0.00001 0.00001 0.00002 -0.01015

D9 0.02323 -0.00001 0.00014 -0.00008 0.00006 0.02329

D10 -3.10550 -0.00001 0.00010 -0.00013 -0.00003 -3.10553

D11 -0.00966 0.00000 -0.00004 0.00001 -0.00003 -0.00969

D12 3.11487 0.00000 -0.00003 0.00003 0.00001 3.11487

D13 2.97168 0.00000 0.00030 0.00011 0.00041 2.97208

D14 -0.18698 0.00001 0.00031 0.00013 0.00044 -0.18654

D15 -3.05826 -0.00001 -0.00002 -0.00009 -0.00011 -3.05837

D16 -0.26560 0.00001 0.00034 0.00022 0.00056 -0.26504

D17 -1.66374 0.00000 0.00016 0.00007 0.00023 -1.66351

D18 0.26640 -0.00001 -0.00040 -0.00020 -0.00060 0.26580

D19 3.05906 0.00001 -0.00003 0.00010 0.00007 3.05913

D20 1.66092 0.00000 -0.00021 -0.00005 -0.00026 1.66066

D21 0.00617 0.00000 0.00001 -0.00004 -0.00003 0.00615

D22 3.13972 0.00000 0.00001 0.00001 0.00002 3.13974

D23 -3.11888 0.00000 0.00000 -0.00006 -0.00006 -3.11894

D24 0.01467 0.00000 0.00000 -0.00002 -0.00001 0.01466

D25 -0.01191 0.00001 -0.00003 0.00004 0.00001 -0.01191

D26 3.10990 0.00001 -0.00002 0.00007 0.00005 3.10995

D27 -0.00077 0.00000 0.00002 0.00005 0.00007 -0.00070

D28 3.13608 0.00000 0.00000 0.00004 0.00004 3.13613

D29 -3.13555 0.00000 0.00002 0.00001 0.00003 -3.13552

D30 0.00131 0.00000 0.00000 0.00001 0.00000 0.00131

D31 -3.13778 0.00000 -0.00002 -0.00001 -0.00004 -3.13781

D32 0.00537 0.00000 0.00000 -0.00004 -0.00004 0.00533

D33 -0.00512 0.00000 -0.00002 0.00004 0.00002 -0.00510

D34 3.13803 0.00000 0.00000 0.00001 0.00001 3.13804

D35 3.13885 0.00000 -0.00001 -0.00005 -0.00006 3.13879

D36 -0.00389 0.00000 -0.00002 0.00000 -0.00001 -0.00390

D37 0.00341 0.00000 0.00002 -0.00005 -0.00002 0.00338

D38 -3.13933 0.00000 0.00001 0.00001 0.00002 -3.13931

D39 0.01191 -0.00001 0.00003 -0.00004 -0.00001 0.01191

D40 -3.10990 -0.00001 0.00002 -0.00007 -0.00005 -3.10995

D41 -3.11487 0.00000 0.00003 -0.00003 -0.00001 -3.11487

D42 0.18698 -0.00001 -0.00031 -0.00013 -0.00044 0.18654

D43 0.00966 0.00000 0.00004 -0.00001 0.00003 0.00969

D44 -2.97168 0.00000 -0.00030 -0.00011 -0.00041 -2.97208

D45 3.11888 0.00000 0.00000 0.00006 0.00006 3.11894

D46 -0.01467 0.00000 0.00000 0.00002 0.00001 -0.01466

D47 -0.00617 0.00000 -0.00001 0.00004 0.00003 -0.00615

D48 -3.13972 0.00000 -0.00001 -0.00001 -0.00002 -3.13974

D49 -0.00917 0.00000 -0.00005 -0.00002 -0.00007 -0.00924

D50 3.12113 0.00000 -0.00002 0.00003 0.00001 3.12113

D51 2.97038 0.00000 0.00029 0.00008 0.00037 2.97075

D52 -0.18251 0.00001 0.00032 0.00012 0.00045 -0.18206

D53 -0.26640 0.00001 0.00040 0.00020 0.00060 -0.26580

D54 -1.66092 0.00000 0.00021 0.00005 0.00026 -1.66066

D55 -3.05906 -0.00001 0.00003 -0.00010 -0.00007 -3.05913

D56 3.05826 0.00001 0.00002 0.00009 0.00011 3.05837

D57 1.66374 0.00000 -0.00016 -0.00007 -0.00023 1.66351

D58 0.26560 -0.00001 -0.00034 -0.00022 -0.00056 0.26504

D59 0.00502 0.00000 0.00005 0.00004 0.00009 0.00511

D60 3.14111 0.00000 0.00002 0.00004 0.00006 3.14117

D61 -3.12592 0.00000 0.00002 0.00000 0.00001 -3.12591

D62 0.01016 0.00000 -0.00001 -0.00001 -0.00002 0.01015

D63 -0.02323 0.00001 -0.00014 0.00008 -0.00006 -0.02329

D64 3.10550 0.00001 -0.00010 0.00013 0.00003 3.10553

D65 0.00077 0.00000 -0.00002 -0.00005 -0.00007 0.00070

D66 3.13555 0.00000 -0.00002 -0.00001 -0.00003 3.13552

D67 -3.13608 0.00000 0.00000 -0.00004 -0.00004 -3.13613

D68 -0.00131 0.00000 0.00000 -0.00001 0.00000 -0.00131

D69 -3.13885 0.00000 0.00001 0.00005 0.00006 -3.13879

D70 0.00389 0.00000 0.00002 0.00000 0.00001 0.00390

D71 -0.00341 0.00000 -0.00002 0.00005 0.00002 -0.00338

D72 3.13933 0.00000 -0.00001 -0.00001 -0.00002 3.13931

D73 3.13778 0.00000 0.00002 0.00001 0.00004 3.13781

D74 -0.00537 0.00000 0.00000 0.00004 0.00004 -0.00533

D75 0.00512 0.00000 0.00002 -0.00004 -0.00002 0.00510

D76 -3.13803 0.00000 0.00000 -0.00001 -0.00001 -3.13804

D77 3.10550 0.00001 -0.00010 0.00013 0.00003 3.10553

D78 -0.02323 0.00001 -0.00014 0.00008 -0.00006 -0.02329

D79 0.00077 0.00000 -0.00002 -0.00005 -0.00007 0.00070

D80 3.13555 0.00000 -0.00002 -0.00001 -0.00003 3.13552

D81 -3.13608 0.00000 0.00000 -0.00004 -0.00004 -3.13613

D82 -0.00131 0.00000 0.00000 -0.00001 0.00000 -0.00131

D83 -3.12592 0.00000 0.00002 0.00000 0.00001 -3.12591

D84 0.00502 0.00000 0.00005 0.00004 0.00009 0.00511

D85 0.01016 0.00000 -0.00001 -0.00001 -0.00002 0.01015

D86 3.14111 0.00000 0.00002 0.00004 0.00006 3.14117

D87 -0.00341 0.00000 -0.00002 0.00005 0.00002 -0.00338

D88 3.13933 0.00000 -0.00001 -0.00001 -0.00002 3.13931

D89 -3.13885 0.00000 0.00001 0.00005 0.00006 -3.13879

D90 0.00389 0.00000 0.00002 0.00000 0.00001 0.00390

D91 -0.00617 0.00000 -0.00001 0.00004 0.00003 -0.00615

D92 3.11888 0.00000 0.00000 0.00006 0.00006 3.11894

D93 -3.13972 0.00000 -0.00001 -0.00001 -0.00002 -3.13974

D94 -0.01467 0.00000 0.00000 0.00002 0.00001 -0.01466

D95 0.00512 0.00000 0.00002 -0.00004 -0.00002 0.00510

D96 -3.13803 0.00000 0.00000 -0.00001 -0.00001 -3.13804

D97 3.13778 0.00000 0.00002 0.00001 0.00004 3.13781

D98 -0.00537 0.00000 0.00000 0.00004 0.00004 -0.00533

D99 0.00966 0.00000 0.00004 -0.00001 0.00003 0.00969

D100 -2.97168 0.00000 -0.00030 -0.00011 -0.00041 -2.97208

D101 -3.11487 0.00000 0.00003 -0.00003 -0.00001 -3.11487

D102 0.18698 -0.00001 -0.00031 -0.00013 -0.00044 0.18654

D103 -3.10990 -0.00001 0.00002 -0.00007 -0.00005 -3.10995

D104 0.01191 -0.00001 0.00003 -0.00004 -0.00001 0.01191

D105 3.12113 0.00000 -0.00002 0.00003 0.00001 3.12113

D106 -0.00917 0.00000 -0.00005 -0.00002 -0.00007 -0.00924

D107 -0.18251 0.00001 0.00032 0.00012 0.00045 -0.18206

D108 2.97038 0.00000 0.00029 0.00008 0.00037 2.97075

D109 -3.05906 -0.00001 0.00003 -0.00010 -0.00007 -3.05913

D110 -1.66092 0.00000 0.00021 0.00005 0.00026 -1.66066

D111 -0.26640 0.00001 0.00040 0.00020 0.00060 -0.26580

D112 0.26560 -0.00001 -0.00034 -0.00022 -0.00056 0.26504

D113 1.66374 0.00000 -0.00016 -0.00007 -0.00023 1.66351

D114 3.05826 0.00001 0.00002 0.00009 0.00011 3.05837

D115 -0.01191 0.00001 -0.00003 0.00004 0.00001 -0.01191

D116 3.10990 0.00001 -0.00002 0.00007 0.00005 3.10995

D117 3.11487 0.00000 -0.00003 0.00003 0.00001 3.11487

D118 -0.00966 0.00000 -0.00004 0.00001 -0.00003 -0.00969

D119 -0.18698 0.00001 0.00031 0.00013 0.00044 -0.18654

D120 2.97168 0.00000 0.00030 0.00011 0.00041 2.97208

D121 0.00917 0.00000 0.00005 0.00002 0.00007 0.00924

D122 -3.12113 0.00000 0.00002 -0.00003 -0.00001 -3.12113

D123 -2.97038 0.00000 -0.00029 -0.00008 -0.00037 -2.97075

D124 0.18251 -0.00001 -0.00032 -0.00012 -0.00045 0.18206

D125 1.66092 0.00000 -0.00021 -0.00005 -0.00026 1.66066

D126 3.05906 0.00001 -0.00003 0.00010 0.00007 3.05913

D127 0.26640 -0.00001 -0.00040 -0.00020 -0.00060 0.26580

D128 -1.66374 0.00000 0.00016 0.00007 0.00023 -1.66351

D129 -0.26560 0.00001 0.00034 0.00022 0.00056 -0.26504

D130 -3.05826 -0.00001 -0.00002 -0.00009 -0.00011 -3.05837

D131 -3.11888 0.00000 0.00000 -0.00006 -0.00006 -3.11894

D132 0.01467 0.00000 0.00000 -0.00002 -0.00001 0.01466

D133 0.00617 0.00000 0.00001 -0.00004 -0.00003 0.00615

D134 3.13972 0.00000 0.00001 0.00001 0.00002 3.13974

D135 -0.00077 0.00000 0.00002 0.00005 0.00007 -0.00070

D136 3.13608 0.00000 0.00000 0.00004 0.00004 3.13613

D137 -3.13555 0.00000 0.00002 0.00001 0.00003 -3.13552

D138 0.00131 0.00000 0.00000 0.00001 0.00000 0.00131

D139 -3.13778 0.00000 -0.00002 -0.00001 -0.00004 -3.13781

D140 0.00537 0.00000 0.00000 -0.00004 -0.00004 0.00533

D141 -0.00512 0.00000 -0.00002 0.00004 0.00002 -0.00510

D142 3.13803 0.00000 0.00000 0.00001 0.00001 3.13804

D143 -0.00502 0.00000 -0.00005 -0.00004 -0.00009 -0.00511

D144 3.12592 0.00000 -0.00002 0.00000 -0.00001 3.12591

D145 -3.14111 0.00000 -0.00002 -0.00004 -0.00006 -3.14117

D146 -0.01016 0.00000 0.00001 0.00001 0.00002 -0.01015

D147 0.00341 0.00000 0.00002 -0.00005 -0.00002 0.00338

D148 -3.13933 0.00000 0.00001 0.00001 0.00002 -3.13931

D149 3.13885 0.00000 -0.00001 -0.00005 -0.00006 3.13879

D150 -0.00389 0.00000 -0.00002 0.00000 -0.00001 -0.00390

D151 0.02323 -0.00001 0.00014 -0.00008 0.00006 0.02329

D152 -3.10550 -0.00001 0.00010 -0.00013 -0.00003 -3.10553

D153 0.00426 0.00000 0.00002 -0.00005 -0.00003 0.00424

D154 -3.13846 0.00000 0.00002 -0.00005 -0.00003 -3.13849

D155 -3.13848 0.00000 0.00001 0.00001 0.00002 -3.13846

D156 0.00198 0.00000 0.00001 0.00000 0.00002 0.00200

D157 -0.00042 0.00000 0.00000 0.00001 0.00001 -0.00041

D158 3.14052 0.00000 0.00001 0.00000 0.00001 3.14053

D159 -3.14088 0.00000 0.00000 0.00001 0.00001 -3.14087

D160 0.00005 0.00000 0.00000 0.00001 0.00001 0.00006

D161 -0.00430 0.00000 -0.00002 0.00004 0.00002 -0.00428

D162 3.13885 0.00000 0.00000 0.00001 0.00001 3.13886

D163 3.13796 0.00000 -0.00003 0.00004 0.00001 3.13797

D164 -0.00208 0.00000 -0.00001 0.00001 0.00001 -0.00207

D165 -0.00426 0.00000 -0.00002 0.00005 0.00003 -0.00424

D166 3.13846 0.00000 -0.00002 0.00005 0.00003 3.13849

D167 3.13848 0.00000 -0.00001 -0.00001 -0.00002 3.13846

D168 -0.00198 0.00000 -0.00001 0.00000 -0.00002 -0.00200

D169 0.00042 0.00000 0.00000 -0.00001 -0.00001 0.00041

D170 -3.14052 0.00000 -0.00001 0.00000 -0.00001 -3.14053

D171 3.14088 0.00000 0.00000 -0.00001 -0.00001 3.14087

D172 -0.00005 0.00000 0.00000 -0.00001 -0.00001 -0.00006

D173 0.00430 0.00000 0.00002 -0.00004 -0.00002 0.00428

D174 -3.13885 0.00000 0.00000 -0.00001 -0.00001 -3.13886

D175 -3.13796 0.00000 0.00003 -0.00004 -0.00001 -3.13797

D176 0.00208 0.00000 0.00001 -0.00001 -0.00001 0.00207

D177 -0.00430 0.00000 -0.00002 0.00004 0.00002 -0.00428

D178 3.13796 0.00000 -0.00003 0.00004 0.00001 3.13797

D179 3.13885 0.00000 0.00000 0.00001 0.00001 3.13886

D180 -0.00208 0.00000 -0.00001 0.00001 0.00001 -0.00207

D181 -0.00042 0.00000 0.00000 0.00001 0.00001 -0.00041

D182 -3.14088 0.00000 0.00000 0.00001 0.00001 -3.14087

D183 3.14052 0.00000 0.00001 0.00000 0.00001 3.14053

D184 0.00005 0.00000 0.00000 0.00001 0.00001 0.00006

D185 0.00426 0.00000 0.00002 -0.00005 -0.00003 0.00424

D186 -3.13848 0.00000 0.00001 0.00001 0.00002 -3.13846

D187 -3.13846 0.00000 0.00002 -0.00005 -0.00003 -3.13849

D188 0.00198 0.00000 0.00001 0.00000 0.00002 0.00200

D189 -0.00426 0.00000 -0.00002 0.00005 0.00003 -0.00424

D190 3.13846 0.00000 -0.00002 0.00005 0.00003 3.13849

D191 3.13848 0.00000 -0.00001 -0.00001 -0.00002 3.13846

D192 -0.00198 0.00000 -0.00001 0.00000 -0.00002 -0.00200

D193 0.00042 0.00000 0.00000 -0.00001 -0.00001 0.00041

D194 -3.14052 0.00000 -0.00001 0.00000 -0.00001 -3.14053

D195 3.14088 0.00000 0.00000 -0.00001 -0.00001 3.14087

D196 -0.00005 0.00000 0.00000 -0.00001 -0.00001 -0.00006

D197 0.00430 0.00000 0.00002 -0.00004 -0.00002 0.00428

D198 -3.13885 0.00000 0.00000 -0.00001 -0.00001 -3.13886

D199 -3.13796 0.00000 0.00003 -0.00004 -0.00001 -3.13797

D200 0.00208 0.00000 0.00001 -0.00001 -0.00001 0.00207

Item Value Threshold Converged?

Maximum Force 0.000023 0.000450 YES

RMS Force 0.000006 0.000300 YES

Maximum Displacement 0.001502 0.001800 YES

RMS Displacement 0.000107 0.001200 YES

Predicted change in Energy=-6.042976D-08

Optimization completed.

-- Stationary point found.

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! Optimized Parameters !

! (Angstroms and Degrees) !

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! Name Definition Value Derivative Info. !

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! R1 R(1,2) 1.3556 -DE/DX = 0.0 !

! R2 R(1,5) 1.4638 -DE/DX = 0.0 !

! R3 R(1,12) 1.3426 -DE/DX = 0.0 !

! R4 R(2,3) 1.3862 -DE/DX = 0.0 !

! R5 R(2,25) 2.0555 -DE/DX = 0.0 !

! R6 R(3,4) 1.4538 -DE/DX = 0.0 !

! R7 R(3,6) 1.3296 -DE/DX = 0.0 !

! R8 R(4,5) 1.4184 -DE/DX = 0.0 !

! R9 R(4,41) 1.3976 -DE/DX = 0.0 !

! R10 R(5,38) 1.3945 -DE/DX = 0.0 !

! R11 R(6,7) 1.3296 -DE/DX = 0.0 !

! R12 R(7,8) 1.3862 -DE/DX = 0.0 !

! R13 R(7,11) 1.4538 -DE/DX = 0.0 !

! R14 R(8,9) 1.3556 -DE/DX = 0.0 !

! R15 R(8,25) 2.0555 -DE/DX = 0.0 !

! R16 R(9,10) 1.4638 -DE/DX = 0.0 !

! R17 R(9,24) 1.3426 -DE/DX = 0.0 !

! R18 R(10,11) 1.4184 -DE/DX = 0.0 !

! R19 R(10,37) 1.3945 -DE/DX = 0.0 !

! R20 R(11,34) 1.3976 -DE/DX = 0.0 !

! R21 R(12,17) 1.3426 -DE/DX = 0.0 !

! R22 R(13,14) 1.4184 -DE/DX = 0.0 !

! R23 R(13,17) 1.4638 -DE/DX = 0.0 !

! R24 R(13,26) 1.3945 -DE/DX = 0.0 !

! R25 R(14,15) 1.4538 -DE/DX = 0.0 !

! R26 R(14,29) 1.3976 -DE/DX = 0.0 !

! R27 R(15,16) 1.3862 -DE/DX = 0.0 !

! R28 R(15,18) 1.3296 -DE/DX = 0.0 !

! R29 R(16,17) 1.3556 -DE/DX = 0.0 !

! R30 R(16,25) 2.0555 -DE/DX = 0.0 !

! R31 R(18,20) 1.3296 -DE/DX = 0.0 !

! R32 R(19,20) 1.3862 -DE/DX = 0.0 !

! R33 R(19,23) 1.3556 -DE/DX = 0.0 !

! R34 R(19,25) 2.0555 -DE/DX = 0.0 !

! R35 R(20,21) 1.4538 -DE/DX = 0.0 !

! R36 R(21,22) 1.4184 -DE/DX = 0.0 !

! R37 R(21,33) 1.3976 -DE/DX = 0.0 !

! R38 R(22,23) 1.4638 -DE/DX = 0.0 !

! R39 R(22,30) 1.3945 -DE/DX = 0.0 !

! R40 R(23,24) 1.3426 -DE/DX = 0.0 !

! R41 R(26,27) 1.3922 -DE/DX = 0.0 !

! R42 R(26,42) 1.0851 -DE/DX = 0.0 !

! R43 R(27,28) 1.4078 -DE/DX = 0.0 !

! R44 R(27,54) 1.0849 -DE/DX = 0.0 !

! R45 R(28,29) 1.3911 -DE/DX = 0.0 !

! R46 R(28,55) 1.0852 -DE/DX = 0.0 !

! R47 R(29,43) 1.0851 -DE/DX = 0.0 !

! R48 R(30,31) 1.3922 -DE/DX = 0.0 !

! R49 R(30,44) 1.0851 -DE/DX = 0.0 !

! R50 R(31,32) 1.4078 -DE/DX = 0.0 !

! R51 R(31,57) 1.0849 -DE/DX = 0.0 !

! R52 R(32,33) 1.3911 -DE/DX = 0.0 !

! R53 R(32,56) 1.0852 -DE/DX = 0.0 !

! R54 R(33,45) 1.0851 -DE/DX = 0.0 !

! R55 R(34,35) 1.3911 -DE/DX = 0.0 !

! R56 R(34,46) 1.0851 -DE/DX = 0.0 !

! R57 R(35,36) 1.4078 -DE/DX = 0.0 !

! R58 R(35,50) 1.0852 -DE/DX = 0.0 !

! R59 R(36,37) 1.3922 -DE/DX = 0.0 !

! R60 R(36,51) 1.0849 -DE/DX = 0.0 !

! R61 R(37,47) 1.0851 -DE/DX = 0.0 !

! R62 R(38,39) 1.3922 -DE/DX = 0.0 !

! R63 R(38,48) 1.0851 -DE/DX = 0.0 !

! R64 R(39,40) 1.4078 -DE/DX = 0.0 !

! R65 R(39,53) 1.0849 -DE/DX = 0.0 !

! R66 R(40,41) 1.3911 -DE/DX = 0.0 !

! R67 R(40,52) 1.0852 -DE/DX = 0.0 !

! R68 R(41,49) 1.0851 -DE/DX = 0.0 !

! A1 A(2,1,5) 108.2785 -DE/DX = 0.0 !

! A2 A(2,1,12) 128.2024 -DE/DX = 0.0 !

! A3 A(5,1,12) 123.5158 -DE/DX = 0.0 !

! A4 A(1,2,3) 110.5469 -DE/DX = 0.0 !

! A5 A(1,2,25) 124.8388 -DE/DX = 0.0 !

! A6 A(3,2,25) 123.9163 -DE/DX = 0.0 !

! A7 A(2,3,4) 107.9084 -DE/DX = 0.0 !

! A8 A(2,3,6) 127.2722 -DE/DX = 0.0 !

! A9 A(4,3,6) 124.8117 -DE/DX = 0.0 !

! A10 A(3,4,5) 106.6113 -DE/DX = 0.0 !

! A11 A(3,4,41) 133.0061 -DE/DX = 0.0 !

! A12 A(5,4,41) 120.381 -DE/DX = 0.0 !

! A13 A(1,5,4) 106.6519 -DE/DX = 0.0 !

! A14 A(1,5,38) 132.4143 -DE/DX = 0.0 !

! A15 A(4,5,38) 120.9331 -DE/DX = 0.0 !

! A16 A(3,6,7) 126.3702 -DE/DX = 0.0 !

! A17 A(6,7,8) 127.2722 -DE/DX = 0.0 !

! A18 A(6,7,11) 124.8117 -DE/DX = 0.0 !

! A19 A(8,7,11) 107.9084 -DE/DX = 0.0 !

! A20 A(7,8,9) 110.5469 -DE/DX = 0.0 !

! A21 A(7,8,25) 123.9163 -DE/DX = 0.0 !

! A22 A(9,8,25) 124.8388 -DE/DX = 0.0 !

! A23 A(8,9,10) 108.2785 -DE/DX = 0.0 !

! A24 A(8,9,24) 128.2024 -DE/DX = 0.0 !

! A25 A(10,9,24) 123.5158 -DE/DX = 0.0 !

! A26 A(9,10,11) 106.6519 -DE/DX = 0.0 !

! A27 A(9,10,37) 132.4143 -DE/DX = 0.0 !

! A28 A(11,10,37) 120.9331 -DE/DX = 0.0 !

! A29 A(7,11,10) 106.6113 -DE/DX = 0.0 !

! A30 A(7,11,34) 133.0061 -DE/DX = 0.0 !

! A31 A(10,11,34) 120.381 -DE/DX = 0.0 !

! A32 A(1,12,17) 123.8522 -DE/DX = 0.0 !

! A33 A(14,13,17) 106.6519 -DE/DX = 0.0 !

! A34 A(14,13,26) 120.9331 -DE/DX = 0.0 !

! A35 A(17,13,26) 132.4143 -DE/DX = 0.0 !

! A36 A(13,14,15) 106.6113 -DE/DX = 0.0 !

! A37 A(13,14,29) 120.381 -DE/DX = 0.0 !

! A38 A(15,14,29) 133.0061 -DE/DX = 0.0 !

! A39 A(14,15,16) 107.9084 -DE/DX = 0.0 !

! A40 A(14,15,18) 124.8117 -DE/DX = 0.0 !

! A41 A(16,15,18) 127.2722 -DE/DX = 0.0 !

! A42 A(15,16,17) 110.5469 -DE/DX = 0.0 !

! A43 A(15,16,25) 123.9163 -DE/DX = 0.0 !

! A44 A(17,16,25) 124.8388 -DE/DX = 0.0 !

! A45 A(12,17,13) 123.5158 -DE/DX = 0.0 !

! A46 A(12,17,16) 128.2024 -DE/DX = 0.0 !

! A47 A(13,17,16) 108.2785 -DE/DX = 0.0 !

! A48 A(15,18,20) 126.3702 -DE/DX = 0.0 !

! A49 A(20,19,23) 110.5469 -DE/DX = 0.0 !

! A50 A(20,19,25) 123.9163 -DE/DX = 0.0 !

! A51 A(23,19,25) 124.8388 -DE/DX = 0.0 !

! A52 A(18,20,19) 127.2722 -DE/DX = 0.0 !

! A53 A(18,20,21) 124.8117 -DE/DX = 0.0 !

! A54 A(19,20,21) 107.9084 -DE/DX = 0.0 !

! A55 A(20,21,22) 106.6113 -DE/DX = 0.0 !

! A56 A(20,21,33) 133.0061 -DE/DX = 0.0 !

! A57 A(22,21,33) 120.381 -DE/DX = 0.0 !

! A58 A(21,22,23) 106.6519 -DE/DX = 0.0 !

! A59 A(21,22,30) 120.9331 -DE/DX = 0.0 !

! A60 A(23,22,30) 132.4143 -DE/DX = 0.0 !

! A61 A(19,23,22) 108.2785 -DE/DX = 0.0 !

! A62 A(19,23,24) 128.2024 -DE/DX = 0.0 !

! A63 A(22,23,24) 123.5158 -DE/DX = 0.0 !

! A64 A(9,24,23) 123.8522 -DE/DX = 0.0 !

! A65 A(2,25,8) 88.8078 -DE/DX = 0.0 !

! A66 A(2,25,16) 87.6317 -DE/DX = 0.0 !

! A67 A(2,25,19) 159.6972 -DE/DX = 0.0 !

! A68 A(8,25,16) 159.6972 -DE/DX = 0.0 !

! A69 A(8,25,19) 87.6317 -DE/DX = 0.0 !

! A70 A(16,25,19) 88.8078 -DE/DX = 0.0 !

! A71 A(13,26,27) 118.3245 -DE/DX = 0.0 !

! A72 A(13,26,42) 120.682 -DE/DX = 0.0 !

! A73 A(27,26,42) 120.9935 -DE/DX = 0.0 !

! A74 A(26,27,28) 120.8135 -DE/DX = 0.0 !

! A75 A(26,27,54) 119.8095 -DE/DX = 0.0 !

! A76 A(28,27,54) 119.3769 -DE/DX = 0.0 !

! A77 A(27,28,29) 121.221 -DE/DX = 0.0 !

! A78 A(27,28,55) 119.2116 -DE/DX = 0.0 !

! A79 A(29,28,55) 119.5674 -DE/DX = 0.0 !

! A80 A(14,29,28) 118.3259 -DE/DX = 0.0 !

! A81 A(14,29,43) 120.7665 -DE/DX = 0.0 !

! A82 A(28,29,43) 120.9075 -DE/DX = 0.0 !

! A83 A(22,30,31) 118.3245 -DE/DX = 0.0 !

! A84 A(22,30,44) 120.682 -DE/DX = 0.0 !

! A85 A(31,30,44) 120.9935 -DE/DX = 0.0 !

! A86 A(30,31,32) 120.8135 -DE/DX = 0.0 !

! A87 A(30,31,57) 119.8095 -DE/DX = 0.0 !

! A88 A(32,31,57) 119.3769 -DE/DX = 0.0 !

! A89 A(31,32,33) 121.221 -DE/DX = 0.0 !

! A90 A(31,32,56) 119.2116 -DE/DX = 0.0 !

! A91 A(33,32,56) 119.5674 -DE/DX = 0.0 !

! A92 A(21,33,32) 118.3259 -DE/DX = 0.0 !

! A93 A(21,33,45) 120.7665 -DE/DX = 0.0 !

! A94 A(32,33,45) 120.9075 -DE/DX = 0.0 !

! A95 A(11,34,35) 118.3259 -DE/DX = 0.0 !

! A96 A(11,34,46) 120.7665 -DE/DX = 0.0 !

! A97 A(35,34,46) 120.9075 -DE/DX = 0.0 !

! A98 A(34,35,36) 121.221 -DE/DX = 0.0 !

! A99 A(34,35,50) 119.5674 -DE/DX = 0.0 !

! A100 A(36,35,50) 119.2116 -DE/DX = 0.0 !

! A101 A(35,36,37) 120.8135 -DE/DX = 0.0 !

! A102 A(35,36,51) 119.3769 -DE/DX = 0.0 !

! A103 A(37,36,51) 119.8095 -DE/DX = 0.0 !

! A104 A(10,37,36) 118.3245 -DE/DX = 0.0 !

! A105 A(10,37,47) 120.682 -DE/DX = 0.0 !

! A106 A(36,37,47) 120.9935 -DE/DX = 0.0 !

! A107 A(5,38,39) 118.3245 -DE/DX = 0.0 !

! A108 A(5,38,48) 120.682 -DE/DX = 0.0 !

! A109 A(39,38,48) 120.9935 -DE/DX = 0.0 !

! A110 A(38,39,40) 120.8135 -DE/DX = 0.0 !

! A111 A(38,39,53) 119.8095 -DE/DX = 0.0 !

! A112 A(40,39,53) 119.3769 -DE/DX = 0.0 !

! A113 A(39,40,41) 121.221 -DE/DX = 0.0 !

! A114 A(39,40,52) 119.2116 -DE/DX = 0.0 !

! A115 A(41,40,52) 119.5674 -DE/DX = 0.0 !

! A116 A(4,41,40) 118.3259 -DE/DX = 0.0 !

! A117 A(4,41,49) 120.7665 -DE/DX = 0.0 !

! A118 A(40,41,49) 120.9075 -DE/DX = 0.0 !

! D1 D(5,1,2,3) 0.5252 -DE/DX = 0.0 !

! D2 D(5,1,2,25) -170.1905 -DE/DX = 0.0 !

! D3 D(12,1,2,3) -178.8274 -DE/DX = 0.0 !

! D4 D(12,1,2,25) 10.4569 -DE/DX = 0.0 !

! D5 D(2,1,5,4) -0.2876 -DE/DX = 0.0 !

! D6 D(2,1,5,38) -179.9721 -DE/DX = 0.0 !

! D7 D(12,1,5,4) 179.1022 -DE/DX = 0.0 !

! D8 D(12,1,5,38) -0.5823 -DE/DX = 0.0 !

! D9 D(2,1,12,17) 1.3309 -DE/DX = 0.0 !

! D10 D(5,1,12,17) -177.9318 -DE/DX = 0.0 !

! D11 D(1,2,3,4) -0.5537 -DE/DX = 0.0 !

! D12 D(1,2,3,6) 178.4686 -DE/DX = 0.0 !

! D13 D(25,2,3,4) 170.2647 -DE/DX = 0.0 !

! D14 D(25,2,3,6) -10.7131 -DE/DX = 0.0 !

! D15 D(1,2,25,8) -175.2252 -DE/DX = 0.0 !

! D16 D(1,2,25,16) -15.2177 -DE/DX = 0.0 !

! D17 D(1,2,25,19) -95.3251 -DE/DX = 0.0 !

! D18 D(3,2,25,8) 15.2636 -DE/DX = 0.0 !

! D19 D(3,2,25,16) 175.2712 -DE/DX = 0.0 !

! D20 D(3,2,25,19) 95.1637 -DE/DX = 0.0 !

! D21 D(2,3,4,5) 0.3538 -DE/DX = 0.0 !

! D22 D(2,3,4,41) 179.893 -DE/DX = 0.0 !

! D23 D(6,3,4,5) -178.6986 -DE/DX = 0.0 !

! D24 D(6,3,4,41) 0.8406 -DE/DX = 0.0 !

! D25 D(2,3,6,7) -0.6826 -DE/DX = 0.0 !

! D26 D(4,3,6,7) 178.1842 -DE/DX = 0.0 !

! D27 D(3,4,5,1) -0.0443 -DE/DX = 0.0 !

! D28 D(3,4,5,38) 179.6842 -DE/DX = 0.0 !

! D29 D(41,4,5,1) -179.6537 -DE/DX = 0.0 !

! D30 D(41,4,5,38) 0.0748 -DE/DX = 0.0 !

! D31 D(3,4,41,40) -179.7813 -DE/DX = 0.0 !

! D32 D(3,4,41,49) 0.3077 -DE/DX = 0.0 !

! D33 D(5,4,41,40) -0.2931 -DE/DX = 0.0 !

! D34 D(5,4,41,49) 179.7958 -DE/DX = 0.0 !

! D35 D(1,5,38,39) 179.8429 -DE/DX = 0.0 !

! D36 D(1,5,38,48) -0.2226 -DE/DX = 0.0 !

! D37 D(4,5,38,39) 0.1952 -DE/DX = 0.0 !

! D38 D(4,5,38,48) -179.8703 -DE/DX = 0.0 !

! D39 D(3,6,7,8) 0.6826 -DE/DX = 0.0 !

! D40 D(3,6,7,11) -178.1842 -DE/DX = 0.0 !

! D41 D(6,7,8,9) -178.4686 -DE/DX = 0.0 !

! D42 D(6,7,8,25) 10.7131 -DE/DX = 0.0 !

! D43 D(11,7,8,9) 0.5537 -DE/DX = 0.0 !

! D44 D(11,7,8,25) -170.2647 -DE/DX = 0.0 !

! D45 D(6,7,11,10) 178.6986 -DE/DX = 0.0 !

! D46 D(6,7,11,34) -0.8406 -DE/DX = 0.0 !

! D47 D(8,7,11,10) -0.3538 -DE/DX = 0.0 !

! D48 D(8,7,11,34) -179.893 -DE/DX = 0.0 !

! D49 D(7,8,9,10) -0.5252 -DE/DX = 0.0 !

! D50 D(7,8,9,24) 178.8274 -DE/DX = 0.0 !

! D51 D(25,8,9,10) 170.1905 -DE/DX = 0.0 !

! D52 D(25,8,9,24) -10.4569 -DE/DX = 0.0 !

! D53 D(7,8,25,2) -15.2636 -DE/DX = 0.0 !

! D54 D(7,8,25,16) -95.1637 -DE/DX = 0.0 !

! D55 D(7,8,25,19) -175.2712 -DE/DX = 0.0 !

! D56 D(9,8,25,2) 175.2252 -DE/DX = 0.0 !

! D57 D(9,8,25,16) 95.3251 -DE/DX = 0.0 !

! D58 D(9,8,25,19) 15.2177 -DE/DX = 0.0 !

! D59 D(8,9,10,11) 0.2876 -DE/DX = 0.0 !

! D60 D(8,9,10,37) 179.9721 -DE/DX = 0.0 !

! D61 D(24,9,10,11) -179.1022 -DE/DX = 0.0 !

! D62 D(24,9,10,37) 0.5823 -DE/DX = 0.0 !

! D63 D(8,9,24,23) -1.3309 -DE/DX = 0.0 !

! D64 D(10,9,24,23) 177.9318 -DE/DX = 0.0 !

! D65 D(9,10,11,7) 0.0443 -DE/DX = 0.0 !

! D66 D(9,10,11,34) 179.6537 -DE/DX = 0.0 !

! D67 D(37,10,11,7) -179.6842 -DE/DX = 0.0 !

! D68 D(37,10,11,34) -0.0748 -DE/DX = 0.0 !

! D69 D(9,10,37,36) -179.8429 -DE/DX = 0.0 !

! D70 D(9,10,37,47) 0.2226 -DE/DX = 0.0 !

! D71 D(11,10,37,36) -0.1952 -DE/DX = 0.0 !

! D72 D(11,10,37,47) 179.8703 -DE/DX = 0.0 !

! D73 D(7,11,34,35) 179.7813 -DE/DX = 0.0 !

! D74 D(7,11,34,46) -0.3077 -DE/DX = 0.0 !

! D75 D(10,11,34,35) 0.2931 -DE/DX = 0.0 !

! D76 D(10,11,34,46) -179.7958 -DE/DX = 0.0 !

! D77 D(1,12,17,13) 177.9318 -DE/DX = 0.0 !

! D78 D(1,12,17,16) -1.3309 -DE/DX = 0.0 !

! D79 D(17,13,14,15) 0.0443 -DE/DX = 0.0 !

! D80 D(17,13,14,29) 179.6537 -DE/DX = 0.0 !

! D81 D(26,13,14,15) -179.6842 -DE/DX = 0.0 !

! D82 D(26,13,14,29) -0.0748 -DE/DX = 0.0 !

! D83 D(14,13,17,12) -179.1022 -DE/DX = 0.0 !

! D84 D(14,13,17,16) 0.2876 -DE/DX = 0.0 !

! D85 D(26,13,17,12) 0.5823 -DE/DX = 0.0 !

! D86 D(26,13,17,16) 179.9721 -DE/DX = 0.0 !

! D87 D(14,13,26,27) -0.1952 -DE/DX = 0.0 !

! D88 D(14,13,26,42) 179.8703 -DE/DX = 0.0 !

! D89 D(17,13,26,27) -179.8429 -DE/DX = 0.0 !

! D90 D(17,13,26,42) 0.2226 -DE/DX = 0.0 !

! D91 D(13,14,15,16) -0.3538 -DE/DX = 0.0 !

! D92 D(13,14,15,18) 178.6986 -DE/DX = 0.0 !

! D93 D(29,14,15,16) -179.893 -DE/DX = 0.0 !

! D94 D(29,14,15,18) -0.8406 -DE/DX = 0.0 !

! D95 D(13,14,29,28) 0.2931 -DE/DX = 0.0 !

! D96 D(13,14,29,43) -179.7958 -DE/DX = 0.0 !

! D97 D(15,14,29,28) 179.7813 -DE/DX = 0.0 !

! D98 D(15,14,29,43) -0.3077 -DE/DX = 0.0 !

! D99 D(14,15,16,17) 0.5537 -DE/DX = 0.0 !

! D100 D(14,15,16,25) -170.2647 -DE/DX = 0.0 !

! D101 D(18,15,16,17) -178.4686 -DE/DX = 0.0 !

! D102 D(18,15,16,25) 10.7131 -DE/DX = 0.0 !

! D103 D(14,15,18,20) -178.1842 -DE/DX = 0.0 !

! D104 D(16,15,18,20) 0.6826 -DE/DX = 0.0 !

! D105 D(15,16,17,12) 178.8274 -DE/DX = 0.0 !

! D106 D(15,16,17,13) -0.5252 -DE/DX = 0.0 !

! D107 D(25,16,17,12) -10.4569 -DE/DX = 0.0 !

! D108 D(25,16,17,13) 170.1905 -DE/DX = 0.0 !

! D109 D(15,16,25,2) -175.2712 -DE/DX = 0.0 !

! D110 D(15,16,25,8) -95.1637 -DE/DX = 0.0 !

! D111 D(15,16,25,19) -15.2636 -DE/DX = 0.0 !

! D112 D(17,16,25,2) 15.2177 -DE/DX = 0.0 !

! D113 D(17,16,25,8) 95.3251 -DE/DX = 0.0 !

! D114 D(17,16,25,19) 175.2252 -DE/DX = 0.0 !

! D115 D(15,18,20,19) -0.6826 -DE/DX = 0.0 !

! D116 D(15,18,20,21) 178.1842 -DE/DX = 0.0 !

! D117 D(23,19,20,18) 178.4686 -DE/DX = 0.0 !

! D118 D(23,19,20,21) -0.5537 -DE/DX = 0.0 !

! D119 D(25,19,20,18) -10.7131 -DE/DX = 0.0 !

! D120 D(25,19,20,21) 170.2647 -DE/DX = 0.0 !

! D121 D(20,19,23,22) 0.5252 -DE/DX = 0.0 !

! D122 D(20,19,23,24) -178.8274 -DE/DX = 0.0 !

! D123 D(25,19,23,22) -170.1905 -DE/DX = 0.0 !

! D124 D(25,19,23,24) 10.4569 -DE/DX = 0.0 !

! D125 D(20,19,25,2) 95.1637 -DE/DX = 0.0 !

! D126 D(20,19,25,8) 175.2712 -DE/DX = 0.0 !

! D127 D(20,19,25,16) 15.2636 -DE/DX = 0.0 !

! D128 D(23,19,25,2) -95.3251 -DE/DX = 0.0 !

! D129 D(23,19,25,8) -15.2177 -DE/DX = 0.0 !

! D130 D(23,19,25,16) -175.2252 -DE/DX = 0.0 !

! D131 D(18,20,21,22) -178.6986 -DE/DX = 0.0 !

! D132 D(18,20,21,33) 0.8406 -DE/DX = 0.0 !

! D133 D(19,20,21,22) 0.3538 -DE/DX = 0.0 !

! D134 D(19,20,21,33) 179.893 -DE/DX = 0.0 !

! D135 D(20,21,22,23) -0.0443 -DE/DX = 0.0 !

! D136 D(20,21,22,30) 179.6842 -DE/DX = 0.0 !

! D137 D(33,21,22,23) -179.6537 -DE/DX = 0.0 !

! D138 D(33,21,22,30) 0.0748 -DE/DX = 0.0 !

! D139 D(20,21,33,32) -179.7813 -DE/DX = 0.0 !

! D140 D(20,21,33,45) 0.3077 -DE/DX = 0.0 !

! D141 D(22,21,33,32) -0.2931 -DE/DX = 0.0 !

! D142 D(22,21,33,45) 179.7958 -DE/DX = 0.0 !

! D143 D(21,22,23,19) -0.2876 -DE/DX = 0.0 !

! D144 D(21,22,23,24) 179.1022 -DE/DX = 0.0 !

! D145 D(30,22,23,19) -179.9721 -DE/DX = 0.0 !

! D146 D(30,22,23,24) -0.5823 -DE/DX = 0.0 !

! D147 D(21,22,30,31) 0.1952 -DE/DX = 0.0 !

! D148 D(21,22,30,44) -179.8703 -DE/DX = 0.0 !

! D149 D(23,22,30,31) 179.8429 -DE/DX = 0.0 !

! D150 D(23,22,30,44) -0.2226 -DE/DX = 0.0 !

! D151 D(19,23,24,9) 1.3309 -DE/DX = 0.0 !

! D152 D(22,23,24,9) -177.9318 -DE/DX = 0.0 !

! D153 D(13,26,27,28) 0.2442 -DE/DX = 0.0 !

! D154 D(13,26,27,54) -179.8206 -DE/DX = 0.0 !

! D155 D(42,26,27,28) -179.8215 -DE/DX = 0.0 !

! D156 D(42,26,27,54) 0.1137 -DE/DX = 0.0 !

! D157 D(26,27,28,29) -0.0238 -DE/DX = 0.0 !

! D158 D(26,27,28,55) 179.9383 -DE/DX = 0.0 !

! D159 D(54,27,28,29) -179.9593 -DE/DX = 0.0 !

! D160 D(54,27,28,55) 0.0029 -DE/DX = 0.0 !

! D161 D(27,28,29,14) -0.2463 -DE/DX = 0.0 !

! D162 D(27,28,29,43) 179.8428 -DE/DX = 0.0 !

! D163 D(55,28,29,14) 179.7917 -DE/DX = 0.0 !

! D164 D(55,28,29,43) -0.1192 -DE/DX = 0.0 !

! D165 D(22,30,31,32) -0.2442 -DE/DX = 0.0 !

! D166 D(22,30,31,57) 179.8206 -DE/DX = 0.0 !

! D167 D(44,30,31,32) 179.8215 -DE/DX = 0.0 !

! D168 D(44,30,31,57) -0.1137 -DE/DX = 0.0 !

! D169 D(30,31,32,33) 0.0238 -DE/DX = 0.0 !

! D170 D(30,31,32,56) -179.9383 -DE/DX = 0.0 !

! D171 D(57,31,32,33) 179.9593 -DE/DX = 0.0 !

! D172 D(57,31,32,56) -0.0029 -DE/DX = 0.0 !

! D173 D(31,32,33,21) 0.2463 -DE/DX = 0.0 !

! D174 D(31,32,33,45) -179.8428 -DE/DX = 0.0 !

! D175 D(56,32,33,21) -179.7917 -DE/DX = 0.0 !

! D176 D(56,32,33,45) 0.1192 -DE/DX = 0.0 !

! D177 D(11,34,35,36) -0.2463 -DE/DX = 0.0 !

! D178 D(11,34,35,50) 179.7917 -DE/DX = 0.0 !

! D179 D(46,34,35,36) 179.8428 -DE/DX = 0.0 !

! D180 D(46,34,35,50) -0.1192 -DE/DX = 0.0 !

! D181 D(34,35,36,37) -0.0238 -DE/DX = 0.0 !

! D182 D(34,35,36,51) -179.9593 -DE/DX = 0.0 !

! D183 D(50,35,36,37) 179.9383 -DE/DX = 0.0 !

! D184 D(50,35,36,51) 0.0029 -DE/DX = 0.0 !

! D185 D(35,36,37,10) 0.2442 -DE/DX = 0.0 !

! D186 D(35,36,37,47) -179.8215 -DE/DX = 0.0 !

! D187 D(51,36,37,10) -179.8206 -DE/DX = 0.0 !

! D188 D(51,36,37,47) 0.1137 -DE/DX = 0.0 !

! D189 D(5,38,39,40) -0.2442 -DE/DX = 0.0 !

! D190 D(5,38,39,53) 179.8206 -DE/DX = 0.0 !

! D191 D(48,38,39,40) 179.8215 -DE/DX = 0.0 !

! D192 D(48,38,39,53) -0.1137 -DE/DX = 0.0 !

! D193 D(38,39,40,41) 0.0238 -DE/DX = 0.0 !

! D194 D(38,39,40,52) -179.9383 -DE/DX = 0.0 !

! D195 D(53,39,40,41) 179.9593 -DE/DX = 0.0 !

! D196 D(53,39,40,52) -0.0029 -DE/DX = 0.0 !

! D197 D(39,40,41,4) 0.2463 -DE/DX = 0.0 !

! D198 D(39,40,41,49) -179.8428 -DE/DX = 0.0 !

! D199 D(52,40,41,4) -179.7917 -DE/DX = 0.0 !

! D200 D(52,40,41,49) 0.1192 -DE/DX = 0.0 !

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

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Largest change from initial coordinates is atom 51 0.031 Angstoms.

Leave Link 103 at Sat Jun 15 12:23:02 2019, MaxMem= 1342177280 cpu: 11.0

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

Stoichiometry C32H16N8Zn(1-,2)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C32H16N4)]

Deg. of freedom 43

Full point group C2V NOp 4

RotChk: IX=0 Diff= 5.47D-17

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 2.772273 1.184599 0.011272

2 7 0 1.438273 1.423126 0.046118

3 6 0 1.186644 2.785828 0.011707

4 6 0 2.465490 3.475468 -0.036881

5 6 0 3.467672 2.471738 -0.038040

6 7 0 0.000000 3.385559 0.002346

7 6 0 -1.186644 2.785828 0.011707

8 7 0 -1.438273 1.423126 0.046118

9 6 0 -2.772273 1.184599 0.011272

10 6 0 -3.467672 2.471738 -0.038040

11 6 0 -2.465490 3.475468 -0.036881

12 7 0 3.404078 0.000000 0.006486

13 6 0 3.467672 -2.471738 -0.038040

14 6 0 2.465490 -3.475468 -0.036881

15 6 0 1.186644 -2.785828 0.011707

16 7 0 1.438273 -1.423126 0.046118

17 6 0 2.772273 -1.184599 0.011272

18 7 0 0.000000 -3.385559 0.002346

19 7 0 -1.438273 -1.423126 0.046118

20 6 0 -1.186644 -2.785828 0.011707

21 6 0 -2.465490 -3.475468 -0.036881

22 6 0 -3.467672 -2.471738 -0.038040

23 6 0 -2.772273 -1.184599 0.011272

24 7 0 -3.404078 0.000000 0.006486

25 30 0 0.000000 0.000000 0.408403

26 6 0 4.819867 -2.808971 -0.086640

27 6 0 5.163187 -4.157451 -0.129918

28 6 0 4.169683 -5.154917 -0.129873

29 6 0 2.818508 -4.826834 -0.086274

30 6 0 -4.819867 -2.808971 -0.086640

31 6 0 -5.163187 -4.157451 -0.129918

32 6 0 -4.169683 -5.154917 -0.129873

33 6 0 -2.818508 -4.826834 -0.086274

34 6 0 -2.818508 4.826834 -0.086274

35 6 0 -4.169683 5.154917 -0.129873

36 6 0 -5.163187 4.157451 -0.129918

37 6 0 -4.819867 2.808971 -0.086640

38 6 0 4.819867 2.808971 -0.086640

39 6 0 5.163187 4.157451 -0.129918

40 6 0 4.169683 5.154917 -0.129873

41 6 0 2.818508 4.826834 -0.086274

42 1 0 5.583123 -2.037692 -0.089448

43 1 0 2.056911 -5.599739 -0.089010

44 1 0 -5.583123 -2.037692 -0.089448

45 1 0 -2.056911 -5.599739 -0.089010

46 1 0 -2.056911 5.599739 -0.089010

47 1 0 -5.583123 2.037692 -0.089448

48 1 0 5.583123 2.037692 -0.089448

49 1 0 2.056911 5.599739 -0.089010

50 1 0 -4.466568 6.198153 -0.165178

51 1 0 -6.208147 4.447087 -0.165237

52 1 0 4.466568 6.198153 -0.165178

53 1 0 6.208147 4.447087 -0.165237

54 1 0 6.208147 -4.447087 -0.165237

55 1 0 4.466568 -6.198153 -0.165178

56 1 0 -4.466568 -6.198153 -0.165178

57 1 0 -6.208147 -4.447087 -0.165237

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Rotational constants (GHZ): 0.0880319 0.0879157 0.0440907

Leave Link 202 at Sat Jun 15 12:23:03 2019, MaxMem= 1342177280 cpu: 3.1

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

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

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Population analysis using the SCF density.

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Orbital symmetries:

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The electronic state is 2-B1.

Alpha occ. eigenvalues -- -14.30461 -14.30461 -14.29732 -14.29732 -14.29732

Alpha occ. eigenvalues -- -14.29732 -14.29148 -14.29147 -10.23122 -10.23122

Alpha occ. eigenvalues -- -10.23122 -10.23122 -10.22296 -10.22296 -10.22296

Alpha occ. eigenvalues -- -10.22296 -10.17267 -10.17267 -10.17267 -10.17267

Alpha occ. eigenvalues -- -10.17202 -10.17201 -10.17201 -10.17201 -10.17140

Alpha occ. eigenvalues -- -10.17139 -10.17139 -10.17139 -10.17011 -10.17011

Alpha occ. eigenvalues -- -10.17011 -10.17011 -10.17002 -10.17002 -10.17002

Alpha occ. eigenvalues -- -10.17001 -10.16850 -10.16850 -10.16850 -10.16850

Alpha occ. eigenvalues -- -0.98706 -0.97352 -0.97337 -0.94680 -0.92521

Alpha occ. eigenvalues -- -0.88821 -0.88259 -0.85726 -0.84614 -0.84610

Alpha occ. eigenvalues -- -0.84573 -0.84257 -0.76486 -0.75246 -0.75158

Alpha occ. eigenvalues -- -0.74993 -0.74756 -0.74698 -0.74645 -0.74497

Alpha occ. eigenvalues -- -0.70964 -0.68423 -0.67777 -0.62853 -0.62470

Alpha occ. eigenvalues -- -0.61925 -0.61901 -0.61611 -0.60902 -0.58665

Alpha occ. eigenvalues -- -0.58546 -0.58110 -0.57725 -0.56773 -0.55772

Alpha occ. eigenvalues -- -0.55279 -0.55246 -0.54143 -0.53866 -0.53811

Alpha occ. eigenvalues -- -0.53659 -0.51859 -0.51553 -0.51418 -0.48647

Alpha occ. eigenvalues -- -0.48399 -0.47106 -0.47083 -0.46273 -0.45671

Alpha occ. eigenvalues -- -0.45669 -0.45272 -0.45230 -0.44888 -0.43400

Alpha occ. eigenvalues -- -0.43352 -0.43341 -0.43241 -0.43234 -0.43198

Alpha occ. eigenvalues -- -0.42118 -0.41613 -0.41468 -0.40898 -0.40826

Alpha occ. eigenvalues -- -0.37366 -0.37309 -0.36378 -0.36073 -0.36007

Alpha occ. eigenvalues -- -0.35943 -0.35915 -0.35795 -0.35280 -0.34535

Alpha occ. eigenvalues -- -0.34018 -0.33918 -0.33872 -0.33307 -0.31661

Alpha occ. eigenvalues -- -0.31620 -0.31083 -0.30984 -0.29510 -0.27496

Alpha occ. eigenvalues -- -0.26774 -0.26601 -0.25583 -0.25478 -0.25373

Alpha occ. eigenvalues -- -0.25010 -0.24981 -0.24861 -0.24239 -0.24184

Alpha occ. eigenvalues -- -0.24170 -0.23976 -0.18115 -0.12791

Alpha virt. eigenvalues -- -0.09006 -0.04265 -0.02618 -0.02158 -0.01921

Alpha virt. eigenvalues -- -0.01847 0.02694 0.02822 0.03140 0.03142

Alpha virt. eigenvalues -- 0.05261 0.05269 0.05862 0.05871 0.06207

Alpha virt. eigenvalues -- 0.07099 0.07101 0.07152 0.07281 0.07710

Alpha virt. eigenvalues -- 0.09095 0.09108 0.10054 0.10783 0.11761

Alpha virt. eigenvalues -- 0.11826 0.12102 0.12109 0.12730 0.13098

Alpha virt. eigenvalues -- 0.14689 0.15358 0.15495 0.16279 0.17663

Alpha virt. eigenvalues -- 0.18239 0.18311 0.18375 0.19642 0.20751

Alpha virt. eigenvalues -- 0.20906 0.21678 0.22170 0.22300 0.23126

Alpha virt. eigenvalues -- 0.24247 0.24256 0.24428 0.24721 0.25284

Alpha virt. eigenvalues -- 0.25560 0.25955 0.27116 0.27177 0.27686

Alpha virt. eigenvalues -- 0.27759 0.28084 0.28251 0.28942 0.28954

Alpha virt. eigenvalues -- 0.29011 0.29070 0.29512 0.30494 0.30747

Alpha virt. eigenvalues -- 0.31093 0.31118 0.32423 0.33356 0.33580

Alpha virt. eigenvalues -- 0.34309 0.34821 0.35724 0.35745 0.36386

Alpha virt. eigenvalues -- 0.36619 0.37092 0.37369 0.38134 0.38207

Alpha virt. eigenvalues -- 0.38774 0.39263 0.39273 0.39918 0.39928

Alpha virt. eigenvalues -- 0.40216 0.40929 0.41035 0.41052 0.41115

Alpha virt. eigenvalues -- 0.41338 0.41761 0.42048 0.42297 0.42606

Alpha virt. eigenvalues -- 0.42747 0.42992 0.43068 0.43110 0.43601

Alpha virt. eigenvalues -- 0.43603 0.43648 0.43649 0.43735 0.43757

Alpha virt. eigenvalues -- 0.43839 0.43964 0.44261 0.44392 0.45905

Alpha virt. eigenvalues -- 0.46040 0.47062 0.47201 0.47424 0.47494

Alpha virt. eigenvalues -- 0.47922 0.47958 0.48267 0.48490 0.48957

Alpha virt. eigenvalues -- 0.50349 0.50473 0.50771 0.51216 0.51599

Alpha virt. eigenvalues -- 0.51695 0.51990 0.52050 0.52326 0.52418

Alpha virt. eigenvalues -- 0.52538 0.53826 0.54483 0.54542 0.54738

Alpha virt. eigenvalues -- 0.55206 0.56274 0.56297 0.57270 0.59028

Alpha virt. eigenvalues -- 0.60314 0.60514 0.60871 0.60880 0.60933

Alpha virt. eigenvalues -- 0.61051 0.61058 0.61450 0.61508 0.61525

Alpha virt. eigenvalues -- 0.61978 0.62370 0.62456 0.63383 0.63508

Alpha virt. eigenvalues -- 0.63519 0.63639 0.64193 0.64985 0.65133

Alpha virt. eigenvalues -- 0.65314 0.65379 0.65436 0.66665 0.67307

Alpha virt. eigenvalues -- 0.67491 0.67603 0.68148 0.68200 0.69982

Alpha virt. eigenvalues -- 0.70423 0.70464 0.70762 0.71079 0.71245

Alpha virt. eigenvalues -- 0.71471 0.72382 0.72673 0.73843 0.74087

Alpha virt. eigenvalues -- 0.74421 0.74722 0.75168 0.75474 0.76760

Alpha virt. eigenvalues -- 0.77624 0.77953 0.77957 0.78118 0.78251

Alpha virt. eigenvalues -- 0.78743 0.78877 0.79768 0.80395 0.80449

Alpha virt. eigenvalues -- 0.80521 0.80563 0.80876 0.82014 0.82498

Alpha virt. eigenvalues -- 0.82551 0.82573 0.83549 0.83913 0.84709

Alpha virt. eigenvalues -- 0.84852 0.86814 0.87070 0.87329 0.87442

Alpha virt. eigenvalues -- 0.87579 0.88851 0.89382 0.89499 0.90168

Alpha virt. eigenvalues -- 0.90727 0.91278 0.91554 0.91789 0.92011

Alpha virt. eigenvalues -- 0.92762 0.92942 0.93259 0.94589 0.95204

Alpha virt. eigenvalues -- 0.96660 0.98142 0.99726 0.99808 0.99862

Alpha virt. eigenvalues -- 1.00286 1.00513 1.00566 1.00662 1.01210

Alpha virt. eigenvalues -- 1.02748 1.02779 1.02967 1.03740 1.03813

Alpha virt. eigenvalues -- 1.06295 1.06405 1.06563 1.07613 1.10875

Alpha virt. eigenvalues -- 1.11275 1.11394 1.11500 1.11671 1.12133

Alpha virt. eigenvalues -- 1.12572 1.12677 1.12950 1.14316 1.14521

Alpha virt. eigenvalues -- 1.14982 1.15035 1.15306 1.15531 1.16267

Alpha virt. eigenvalues -- 1.17294 1.19187 1.19955 1.21191 1.21357

Alpha virt. eigenvalues -- 1.21374 1.21564 1.21666 1.21742 1.21756

Alpha virt. eigenvalues -- 1.21780 1.23643 1.23807 1.26013 1.26202

Alpha virt. eigenvalues -- 1.26336 1.26801 1.27566 1.27611 1.27762

Alpha virt. eigenvalues -- 1.28753 1.29295 1.29794 1.30251 1.32717

Alpha virt. eigenvalues -- 1.34700 1.34766 1.34928 1.35343 1.35610

Alpha virt. eigenvalues -- 1.36268 1.39195 1.39797 1.42310 1.42339

Alpha virt. eigenvalues -- 1.42837 1.43316 1.43596 1.43606 1.45705

Alpha virt. eigenvalues -- 1.46013 1.46066 1.46080 1.46148 1.46204

Alpha virt. eigenvalues -- 1.49078 1.50450 1.51785 1.51883 1.52444

Alpha virt. eigenvalues -- 1.53432 1.53550 1.53631 1.53842 1.53844

Alpha virt. eigenvalues -- 1.54287 1.54389 1.55654 1.56382 1.58509

Alpha virt. eigenvalues -- 1.58529 1.60377 1.62859 1.62896 1.63327

Alpha virt. eigenvalues -- 1.63614 1.64248 1.65427 1.66421 1.66636

Alpha virt. eigenvalues -- 1.67162 1.68225 1.69094 1.69356 1.72778

Alpha virt. eigenvalues -- 1.72882 1.73159 1.74766 1.74892 1.74973

Alpha virt. eigenvalues -- 1.75115 1.75479 1.76236 1.76272 1.76345

Alpha virt. eigenvalues -- 1.81712 1.81829 1.81909 1.81960 1.82501

Alpha virt. eigenvalues -- 1.83021 1.83251 1.83690 1.83717 1.84172

Alpha virt. eigenvalues -- 1.85009 1.85191 1.85480 1.87243 1.87422

Alpha virt. eigenvalues -- 1.87779 1.89699 1.90560 1.91374 1.91510

Alpha virt. eigenvalues -- 1.91539 1.91648 1.91663 1.91883 1.91904

Alpha virt. eigenvalues -- 1.91921 1.92145 1.92661 1.92989 1.93088

Alpha virt. eigenvalues -- 1.93507 1.93705 1.94621 1.95530 1.95908

Alpha virt. eigenvalues -- 1.96247 1.97244 1.99539 1.99912 2.00109

Alpha virt. eigenvalues -- 2.00690 2.01993 2.03421 2.03447 2.03956

Alpha virt. eigenvalues -- 2.04557 2.05660 2.06309 2.06410 2.08852

Alpha virt. eigenvalues -- 2.12258 2.14289 2.14330 2.16755 2.16775

Alpha virt. eigenvalues -- 2.18861 2.20006 2.22451 2.23635 2.24083

Alpha virt. eigenvalues -- 2.24372 2.24763 2.25479 2.25944 2.26328

Alpha virt. eigenvalues -- 2.27172 2.27740 2.28200 2.28284 2.28628

Alpha virt. eigenvalues -- 2.28812 2.28880 2.29335 2.29649 2.30769

Alpha virt. eigenvalues -- 2.31113 2.31194 2.31318 2.33408 2.33704

Alpha virt. eigenvalues -- 2.33728 2.34388 2.37952 2.39307 2.39591

Alpha virt. eigenvalues -- 2.40253 2.40399 2.40571 2.41534 2.42479

Alpha virt. eigenvalues -- 2.44243 2.44394 2.44919 2.46218 2.47022

Alpha virt. eigenvalues -- 2.49880 2.49982 2.52844 2.53248 2.54084

Alpha virt. eigenvalues -- 2.54226 2.55441 2.56061 2.56998 2.57396

Alpha virt. eigenvalues -- 2.58422 2.58684 2.59055 2.59173 2.60223

Alpha virt. eigenvalues -- 2.62106 2.65059 2.65471 2.65846 2.66277

Alpha virt. eigenvalues -- 2.66526 2.66946 2.68971 2.69391 2.69515

Alpha virt. eigenvalues -- 2.69585 2.70840 2.74078 2.75037 2.75063

Alpha virt. eigenvalues -- 2.75253 2.75704 2.75792 2.75826 2.76720

Alpha virt. eigenvalues -- 2.78277 2.78411 2.78497 2.79380 2.79816

Alpha virt. eigenvalues -- 2.80176 2.80270 2.82675 2.82974 2.83226

Alpha virt. eigenvalues -- 2.83275 2.83347 2.85094 2.85861 2.86258

Alpha virt. eigenvalues -- 2.87220 2.88851 2.89069 2.89337 2.89891

Alpha virt. eigenvalues -- 2.92600 2.92815 2.92992 2.93143 2.93205

Alpha virt. eigenvalues -- 2.98020 2.98337 3.00864 3.04601 3.05604

Alpha virt. eigenvalues -- 3.05618 3.06233 3.08310 3.09462 3.10575

Alpha virt. eigenvalues -- 3.16786 3.17590 3.17645 3.17847 3.18670

Alpha virt. eigenvalues -- 3.19758 3.20586 3.20681 3.21006 3.22365

Alpha virt. eigenvalues -- 3.23519 3.23818 3.24441 3.27009 3.27168

Alpha virt. eigenvalues -- 3.27502 3.27564 3.28267 3.28362 3.28616

Alpha virt. eigenvalues -- 3.29407 3.31091 3.31513 3.31781 3.31782

Alpha virt. eigenvalues -- 3.31973 3.33966 3.34105 3.37117 3.38695

Alpha virt. eigenvalues -- 3.40806 3.40860 3.42306 3.46788 3.47674

Alpha virt. eigenvalues -- 3.47760 3.48278 3.48538 3.48880 3.48982

Alpha virt. eigenvalues -- 3.50448 3.57058 3.62077 3.62531 3.65642

Alpha virt. eigenvalues -- 3.65669 3.65741 3.66280 3.73211 3.73407

Alpha virt. eigenvalues -- 3.73939 3.75127 3.76364 3.77393 3.77840

Alpha virt. eigenvalues -- 3.78005 3.83466 3.84611 3.84861 3.85325

Alpha virt. eigenvalues -- 3.88285 3.89338 3.90642 3.90980 3.91930

Alpha virt. eigenvalues -- 3.96259 3.97001 3.97029 3.97935 4.11638

Alpha virt. eigenvalues -- 4.12647 4.13290 4.19042 4.19368 4.19465

Alpha virt. eigenvalues -- 4.21522 4.24360 4.35380 4.40889 4.41761

Alpha virt. eigenvalues -- 4.41894 4.47717 4.53485 4.55589 4.55595

Alpha virt. eigenvalues -- 4.79521 4.79688 4.79691 4.80018 5.13444

Alpha virt. eigenvalues -- 5.14239 5.14852 5.17859 5.22018 5.35829

Alpha virt. eigenvalues -- 5.38089 5.53143 7.85768 7.85902 7.86462

Alpha virt. eigenvalues -- 7.92559 8.16141 11.13864 23.28579 23.31646

Alpha virt. eigenvalues -- 23.31661 23.33433 23.77727 23.79384 23.79596

Alpha virt. eigenvalues -- 23.79613 23.79843 23.80068 23.80285 23.81984

Alpha virt. eigenvalues -- 23.89513 23.89797 23.90642 23.90764 23.92006

Alpha virt. eigenvalues -- 23.92078 23.92160 23.92575 24.03811 24.04089

Alpha virt. eigenvalues -- 24.04144 24.04718 24.06515 24.06523 24.06569

Alpha virt. eigenvalues -- 24.06645 24.14429 24.14568 24.14589 24.14919

Alpha virt. eigenvalues -- 35.58212 35.61556 35.62057 35.62804 35.70159

Alpha virt. eigenvalues -- 35.70850 35.70899 35.71032

Beta occ. eigenvalues -- -14.30579 -14.30579 -14.29677 -14.29677 -14.29677

Beta occ. eigenvalues -- -14.29676 -14.28815 -14.28815 -10.23158 -10.23158

Beta occ. eigenvalues -- -10.23158 -10.23157 -10.22063 -10.22063 -10.22063

Beta occ. eigenvalues -- -10.22063 -10.17297 -10.17297 -10.17297 -10.17297

Beta occ. eigenvalues -- -10.17195 -10.17195 -10.17195 -10.17195 -10.17134

Beta occ. eigenvalues -- -10.17134 -10.17134 -10.17134 -10.17031 -10.17031

Beta occ. eigenvalues -- -10.17031 -10.17031 -10.16932 -10.16932 -10.16932

Beta occ. eigenvalues -- -10.16932 -10.16791 -10.16791 -10.16791 -10.16791

Beta occ. eigenvalues -- -0.98482 -0.97158 -0.97086 -0.94491 -0.92261

Beta occ. eigenvalues -- -0.88799 -0.87807 -0.85573 -0.84557 -0.84553

Beta occ. eigenvalues -- -0.84488 -0.84087 -0.76341 -0.75124 -0.75112

Beta occ. eigenvalues -- -0.74905 -0.74702 -0.74610 -0.74560 -0.74405

Beta occ. eigenvalues -- -0.70750 -0.67994 -0.67741 -0.62729 -0.62403

Beta occ. eigenvalues -- -0.61866 -0.61849 -0.61461 -0.60820 -0.58593

Beta occ. eigenvalues -- -0.58471 -0.58003 -0.57654 -0.56760 -0.55757

Beta occ. eigenvalues -- -0.55239 -0.55237 -0.54091 -0.53778 -0.53770

Beta occ. eigenvalues -- -0.53582 -0.51735 -0.51474 -0.51381 -0.48559

Beta occ. eigenvalues -- -0.48294 -0.47055 -0.46964 -0.46238 -0.45632

Beta occ. eigenvalues -- -0.45631 -0.45223 -0.45174 -0.44338 -0.43319

Beta occ. eigenvalues -- -0.43225 -0.43216 -0.43185 -0.42856 -0.42799

Beta occ. eigenvalues -- -0.42076 -0.41560 -0.41437 -0.40856 -0.40419

Beta occ. eigenvalues -- -0.37250 -0.36603 -0.36338 -0.36027 -0.35971

Beta occ. eigenvalues -- -0.35697 -0.35602 -0.35596 -0.35227 -0.34513

Beta occ. eigenvalues -- -0.33883 -0.33850 -0.33720 -0.33279 -0.31518

Beta occ. eigenvalues -- -0.31468 -0.30889 -0.29994 -0.29350 -0.27156

Beta occ. eigenvalues -- -0.26650 -0.26425 -0.25409 -0.25287 -0.25042

Beta occ. eigenvalues -- -0.24881 -0.24861 -0.24623 -0.23951 -0.23767

Beta occ. eigenvalues -- -0.23727 -0.23254 -0.16894

Beta virt. eigenvalues -- -0.09118 -0.08667 -0.03365 -0.02279 -0.01975

Beta virt. eigenvalues -- -0.01688 -0.01629 0.03045 0.03193 0.03323

Beta virt. eigenvalues -- 0.03429 0.05298 0.05299 0.05890 0.06547

Beta virt. eigenvalues -- 0.06833 0.07114 0.07117 0.07159 0.07319

Beta virt. eigenvalues -- 0.07717 0.09099 0.09120 0.10070 0.10790

Beta virt. eigenvalues -- 0.12097 0.12112 0.12513 0.12526 0.12747

Beta virt. eigenvalues -- 0.13618 0.14698 0.15382 0.15498 0.16288

Beta virt. eigenvalues -- 0.17925 0.18551 0.18674 0.18698 0.19780

Beta virt. eigenvalues -- 0.20982 0.20998 0.21690 0.22291 0.22555

Beta virt. eigenvalues -- 0.23370 0.24286 0.24334 0.24692 0.24864

Beta virt. eigenvalues -- 0.25338 0.25636 0.25997 0.27203 0.27292

Beta virt. eigenvalues -- 0.27745 0.27811 0.28119 0.28377 0.29005

Beta virt. eigenvalues -- 0.29008 0.29071 0.29125 0.29552 0.30666

Beta virt. eigenvalues -- 0.30817 0.31141 0.31179 0.32641 0.33428

Beta virt. eigenvalues -- 0.33712 0.34397 0.34844 0.35799 0.35845

Beta virt. eigenvalues -- 0.36534 0.36746 0.37358 0.37436 0.38203

Beta virt. eigenvalues -- 0.38283 0.38848 0.39333 0.39401 0.39997

Beta virt. eigenvalues -- 0.40078 0.40277 0.41040 0.41053 0.41139

Beta virt. eigenvalues -- 0.41176 0.41554 0.41849 0.42162 0.42435

Beta virt. eigenvalues -- 0.42697 0.42806 0.43080 0.43156 0.43165

Beta virt. eigenvalues -- 0.43662 0.43673 0.43712 0.43785 0.43786

Beta virt. eigenvalues -- 0.43926 0.43969 0.44148 0.44300 0.44476

Beta virt. eigenvalues -- 0.45974 0.46094 0.47220 0.47374 0.47452

Beta virt. eigenvalues -- 0.47566 0.47992 0.48054 0.48324 0.48571

Beta virt. eigenvalues -- 0.49018 0.50538 0.50585 0.50883 0.51370

Beta virt. eigenvalues -- 0.51628 0.51788 0.52068 0.52229 0.52457

Beta virt. eigenvalues -- 0.52540 0.52669 0.53896 0.54588 0.54607

Beta virt. eigenvalues -- 0.54861 0.55300 0.56363 0.56418 0.57385

Beta virt. eigenvalues -- 0.59176 0.60410 0.60610 0.60889 0.60930

Beta virt. eigenvalues -- 0.60988 0.61095 0.61102 0.61476 0.61538

Beta virt. eigenvalues -- 0.61783 0.62157 0.62428 0.62520 0.63432

Beta virt. eigenvalues -- 0.63583 0.63632 0.63702 0.64266 0.65042

Beta virt. eigenvalues -- 0.65172 0.65374 0.65459 0.65496 0.66729

Beta virt. eigenvalues -- 0.67398 0.67639 0.67667 0.68252 0.68263

Beta virt. eigenvalues -- 0.70082 0.70515 0.70561 0.70824 0.71306

Beta virt. eigenvalues -- 0.71324 0.71691 0.72528 0.72732 0.73912

Beta virt. eigenvalues -- 0.74131 0.74523 0.74763 0.75302 0.75507

Beta virt. eigenvalues -- 0.76941 0.77648 0.77972 0.78018 0.78188

Beta virt. eigenvalues -- 0.78331 0.78857 0.79220 0.79903 0.80405

Beta virt. eigenvalues -- 0.80566 0.80646 0.80755 0.81041 0.82245

Beta virt. eigenvalues -- 0.82587 0.82619 0.82625 0.83601 0.83940

Beta virt. eigenvalues -- 0.84760 0.84884 0.86897 0.87253 0.87421

Beta virt. eigenvalues -- 0.87571 0.87594 0.88888 0.89457 0.89543

Beta virt. eigenvalues -- 0.90220 0.90779 0.91336 0.91574 0.91876

Beta virt. eigenvalues -- 0.92049 0.92824 0.93095 0.93345 0.94632

Beta virt. eigenvalues -- 0.95279 0.96712 0.98292 0.99792 0.99866

Beta virt. eigenvalues -- 0.99973 1.00405 1.00600 1.00633 1.00715

Beta virt. eigenvalues -- 1.01295 1.02810 1.02819 1.02988 1.03860

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Beta virt. eigenvalues -- 1.14648 1.15145 1.15160 1.15408 1.15705

Beta virt. eigenvalues -- 1.16428 1.17398 1.19558 1.20028 1.21301

Beta virt. eigenvalues -- 1.21434 1.21509 1.21698 1.21702 1.21815

Beta virt. eigenvalues -- 1.21833 1.21870 1.23699 1.23904 1.26057

Beta virt. eigenvalues -- 1.26352 1.26627 1.26870 1.27609 1.27666

Beta virt. eigenvalues -- 1.27829 1.28820 1.29332 1.29873 1.30458

Beta virt. eigenvalues -- 1.32802 1.34830 1.34925 1.35102 1.35473

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Beta virt. eigenvalues -- 1.52508 1.53533 1.53773 1.53805 1.54024

Beta virt. eigenvalues -- 1.54075 1.54352 1.54508 1.55736 1.56516

Beta virt. eigenvalues -- 1.58607 1.58697 1.60539 1.63030 1.63152

Beta virt. eigenvalues -- 1.63461 1.63809 1.64369 1.65502 1.66504

Beta virt. eigenvalues -- 1.66768 1.67254 1.68379 1.69243 1.69443

Beta virt. eigenvalues -- 1.72895 1.73048 1.73241 1.74828 1.74957

Beta virt. eigenvalues -- 1.75059 1.75123 1.75572 1.76288 1.76339

Beta virt. eigenvalues -- 1.76428 1.81829 1.81956 1.81999 1.82016

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Beta virt. eigenvalues -- 3.85512 3.88580 3.89903 3.90986 3.91450

Beta virt. eigenvalues -- 3.92287 3.96302 3.97049 3.97071 3.97980

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Beta virt. eigenvalues -- 4.55710 4.79568 4.79738 4.79741 4.80069

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Beta virt. eigenvalues -- 5.36021 5.38251 5.53323 7.85772 7.85932

Beta virt. eigenvalues -- 7.86460 7.92563 8.16145 11.13874 23.28601

Beta virt. eigenvalues -- 23.31667 23.31683 23.33454 23.77814 23.79399

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Beta virt. eigenvalues -- 24.04114 24.04171 24.04742 24.06530 24.06538

Beta virt. eigenvalues -- 24.06586 24.06661 24.14446 24.14586 24.14606

Beta virt. eigenvalues -- 24.14937 35.58294 35.61658 35.62094 35.62863

Beta virt. eigenvalues -- 35.70247 35.70933 35.71017 35.71158

Condensed to atoms (all electrons):

Atomic-Atomic Spin Densities.

Mulliken charges and spin densities:

1 2

1 C 0.363101 -0.018571

2 N -0.669265 0.022956

3 C 0.319666 0.142611

4 C -0.053399 -0.022438

5 C -0.079973 0.047921

6 N -0.394542 -0.063372

7 C 0.319666 0.142611

8 N -0.669265 0.022956

9 C 0.363101 -0.018571

10 C -0.079973 0.047921

11 C -0.053399 -0.022438

12 N -0.443653 0.150787

13 C -0.079973 0.047921

14 C -0.053399 -0.022438

15 C 0.319666 0.142611

16 N -0.669265 0.022956

17 C 0.363101 -0.018571

18 N -0.394542 -0.063372

19 N -0.669265 0.022956

20 C 0.319666 0.142611

21 C -0.053399 -0.022438

22 C -0.079973 0.047921

23 C 0.363101 -0.018571

24 N -0.443653 0.150787

25 Zn 1.364098 -0.002679

26 C -0.223104 -0.023512

27 C -0.241192 0.044379

28 C -0.233055 -0.018658

29 C -0.230505 0.034780

30 C -0.223104 -0.023512

31 C -0.241192 0.044379

32 C -0.233055 -0.018658

33 C -0.230505 0.034780

34 C -0.230505 0.034780

35 C -0.233055 -0.018658

36 C -0.241192 0.044379

37 C -0.223104 -0.023512

38 C -0.223104 -0.023512

39 C -0.241192 0.044379

40 C -0.233055 -0.018658

41 C -0.230505 0.034780

42 H 0.215635 0.000776

43 H 0.215694 -0.001577

44 H 0.215635 0.000776

45 H 0.215694 -0.001577

46 H 0.215694 -0.001577

47 H 0.215635 0.000776

48 H 0.215635 0.000776

49 H 0.215694 -0.001577

50 H 0.222561 0.000780

51 H 0.221907 -0.002485

52 H 0.222561 0.000780

53 H 0.221907 -0.002485

54 H 0.221907 -0.002485

55 H 0.222561 0.000780

56 H 0.222561 0.000780

57 H 0.221907 -0.002485

Sum of Mulliken charges = -1.00000 1.00000

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

1 2

1 C 0.363101 -0.018571

2 N -0.669265 0.022956

3 C 0.319666 0.142611

4 C -0.053399 -0.022438

5 C -0.079973 0.047921

6 N -0.394542 -0.063372

7 C 0.319666 0.142611

8 N -0.669265 0.022956

9 C 0.363101 -0.018571

10 C -0.079973 0.047921

11 C -0.053399 -0.022438

12 N -0.443653 0.150787

13 C -0.079973 0.047921

14 C -0.053399 -0.022438

15 C 0.319666 0.142611

16 N -0.669265 0.022956

17 C 0.363101 -0.018571

18 N -0.394542 -0.063372

19 N -0.669265 0.022956

20 C 0.319666 0.142611

21 C -0.053399 -0.022438

22 C -0.079973 0.047921

23 C 0.363101 -0.018571

24 N -0.443653 0.150787

25 Zn 1.364098 -0.002679

26 C -0.007469 -0.022736

27 C -0.019284 0.041893

28 C -0.010494 -0.017878

29 C -0.014810 0.033204

30 C -0.007469 -0.022736

31 C -0.019284 0.041893

32 C -0.010494 -0.017878

33 C -0.014810 0.033204

34 C -0.014810 0.033204

35 C -0.010494 -0.017878

36 C -0.019284 0.041893

37 C -0.007469 -0.022736

38 C -0.007469 -0.022736

39 C -0.019284 0.041893

40 C -0.010494 -0.017878

41 C -0.014810 0.033204

Electronic spatial extent (au): <R\*\*2>= 22378.4174

Charge= -1.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 0.0000 Y= 0.0000 Z= 2.1157 Tot= 2.1157

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

XX= -261.0807 YY= -258.1328 ZZ= -247.9716

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

XX= -5.3523 YY= -2.4044 ZZ= 7.7568

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

XXX= 0.0000 YYY= 0.0000 ZZZ= 28.1810 XYY= 0.0000

XXY= 0.0000 XXZ= -2.6723 XZZ= 0.0000 YZZ= 0.0000

YYZ= -2.5590 XYZ= 0.0000

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

XXXX= -14796.8646 YYYY= -14680.5860 ZZZZ= -288.5005 XXXY= 0.0000

XXXZ= 0.0000 YYYX= 0.0000 YYYZ= 0.0000 ZZZX= 0.0000

ZZZY= 0.0000 XXYY= -4716.7449 XXZZ= -2963.2199 YYZZ= -2958.8498

XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= 0.0000

N-N= 4.373820765202D+03 E-N=-1.289479184448D+04 KE= 1.776674872624D+03

Symmetry A1 KE= 5.098465934376D+02

Symmetry A2 KE= 3.906850566463D+02

Symmetry B1 KE= 4.388338743691D+02

Symmetry B2 KE= 4.373093481709D+02

Isotropic Fermi Contact Couplings

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

1 C(13) -0.00730 -8.20194 -2.92665 -2.73587

2 N(14) 0.00055 0.17859 0.06373 0.05957

3 C(13) 0.01057 11.87773 4.23827 3.96199

4 C(13) -0.00692 -7.77795 -2.77537 -2.59444

5 C(13) 0.00321 3.61211 1.28889 1.20487

6 N(14) -0.01147 -3.70517 -1.32210 -1.23591

7 C(13) 0.01057 11.87773 4.23827 3.96199

8 N(14) 0.00055 0.17859 0.06373 0.05957

9 C(13) -0.00730 -8.20194 -2.92665 -2.73587

10 C(13) 0.00321 3.61211 1.28889 1.20487

11 C(13) -0.00692 -7.77795 -2.77537 -2.59444

12 N(14) 0.01772 5.72565 2.04305 1.90987

13 C(13) 0.00321 3.61211 1.28889 1.20487

14 C(13) -0.00692 -7.77795 -2.77537 -2.59444

15 C(13) 0.01057 11.87773 4.23827 3.96199

16 N(14) 0.00055 0.17859 0.06373 0.05957

17 C(13) -0.00730 -8.20194 -2.92665 -2.73587

18 N(14) -0.01147 -3.70517 -1.32210 -1.23591

19 N(14) 0.00055 0.17859 0.06373 0.05957

20 C(13) 0.01057 11.87773 4.23827 3.96199

21 C(13) -0.00692 -7.77795 -2.77537 -2.59444

22 C(13) 0.00321 3.61211 1.28889 1.20487

23 C(13) -0.00730 -8.20194 -2.92665 -2.73587

24 N(14) 0.01772 5.72565 2.04305 1.90987

25 Zn(67) 0.00000 0.00000 0.00000 0.00000

26 C(13) -0.00343 -3.85534 -1.37568 -1.28600

27 C(13) 0.00305 3.43241 1.22477 1.14493

28 C(13) -0.00275 -3.08805 -1.10189 -1.03006

29 C(13) 0.00222 2.49477 0.89020 0.83217

30 C(13) -0.00343 -3.85534 -1.37568 -1.28600

31 C(13) 0.00305 3.43241 1.22477 1.14493

32 C(13) -0.00275 -3.08805 -1.10189 -1.03006

33 C(13) 0.00222 2.49477 0.89020 0.83217

34 C(13) 0.00222 2.49477 0.89020 0.83217

35 C(13) -0.00275 -3.08805 -1.10189 -1.03006

36 C(13) 0.00305 3.43241 1.22477 1.14493

37 C(13) -0.00343 -3.85534 -1.37568 -1.28600

38 C(13) -0.00343 -3.85534 -1.37568 -1.28600

39 C(13) 0.00305 3.43241 1.22477 1.14493

40 C(13) -0.00275 -3.08805 -1.10189 -1.03006

41 C(13) 0.00222 2.49477 0.89020 0.83217

42 H(1) 0.00027 1.20466 0.42985 0.40183

43 H(1) -0.00049 -2.19544 -0.78339 -0.73232

44 H(1) 0.00027 1.20466 0.42985 0.40183

45 H(1) -0.00049 -2.19544 -0.78339 -0.73232

46 H(1) -0.00049 -2.19544 -0.78339 -0.73232

47 H(1) 0.00027 1.20466 0.42985 0.40183

48 H(1) 0.00027 1.20466 0.42985 0.40183

49 H(1) -0.00049 -2.19544 -0.78339 -0.73232

50 H(1) 0.00020 0.88508 0.31582 0.29523

51 H(1) -0.00064 -2.85058 -1.01716 -0.95085

52 H(1) 0.00020 0.88508 0.31582 0.29523

53 H(1) -0.00064 -2.85058 -1.01716 -0.95085

54 H(1) -0.00064 -2.85058 -1.01716 -0.95085

55 H(1) 0.00020 0.88508 0.31582 0.29523

56 H(1) 0.00020 0.88508 0.31582 0.29523

57 H(1) -0.00064 -2.85058 -1.01716 -0.95085

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

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

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1 Atom 0.008494 0.012752 -0.021245

2 Atom -0.034987 -0.036052 0.071038

3 Atom -0.094652 -0.094545 0.189197

4 Atom 0.006783 0.007583 -0.014366

5 Atom -0.027419 -0.027500 0.054919

6 Atom 0.061678 0.046884 -0.108561

7 Atom -0.094652 -0.094545 0.189197

8 Atom -0.034987 -0.036052 0.071038

9 Atom 0.008494 0.012752 -0.021245

10 Atom -0.027419 -0.027500 0.054919

11 Atom 0.006783 0.007583 -0.014366

12 Atom -0.187197 -0.188825 0.376022

13 Atom -0.027419 -0.027500 0.054919

14 Atom 0.006783 0.007583 -0.014366

15 Atom -0.094652 -0.094545 0.189197

16 Atom -0.034987 -0.036052 0.071038

17 Atom 0.008494 0.012752 -0.021245

18 Atom 0.061678 0.046884 -0.108561

19 Atom -0.034987 -0.036052 0.071038

20 Atom -0.094652 -0.094545 0.189197

21 Atom 0.006783 0.007583 -0.014366

22 Atom -0.027419 -0.027500 0.054919

23 Atom 0.008494 0.012752 -0.021245

24 Atom -0.187197 -0.188825 0.376022

25 Atom 0.005698 -0.006920 0.001222

26 Atom 0.011304 0.011071 -0.022375

27 Atom -0.022516 -0.024259 0.046775

28 Atom 0.008949 0.007663 -0.016612

29 Atom -0.017469 -0.016635 0.034103

30 Atom 0.011304 0.011071 -0.022375

31 Atom -0.022516 -0.024259 0.046775

32 Atom 0.008949 0.007663 -0.016612

33 Atom -0.017469 -0.016635 0.034103

34 Atom -0.017469 -0.016635 0.034103

35 Atom 0.008949 0.007663 -0.016612

36 Atom -0.022516 -0.024259 0.046775

37 Atom 0.011304 0.011071 -0.022375

38 Atom 0.011304 0.011071 -0.022375

39 Atom -0.022516 -0.024259 0.046775

40 Atom 0.008949 0.007663 -0.016612

41 Atom -0.017469 -0.016635 0.034103

42 Atom 0.001123 0.000401 -0.001524

43 Atom -0.000146 0.001351 -0.001205

44 Atom 0.001123 0.000401 -0.001524

45 Atom -0.000146 0.001351 -0.001205

46 Atom -0.000146 0.001351 -0.001205

47 Atom 0.001123 0.000401 -0.001524

48 Atom 0.001123 0.000401 -0.001524

49 Atom -0.000146 0.001351 -0.001205

50 Atom 0.000960 -0.000168 -0.000791

51 Atom 0.002883 -0.002387 -0.000497

52 Atom 0.000960 -0.000168 -0.000791

53 Atom 0.002883 -0.002387 -0.000497

54 Atom 0.002883 -0.002387 -0.000497

55 Atom 0.000960 -0.000168 -0.000791

56 Atom 0.000960 -0.000168 -0.000791

57 Atom 0.002883 -0.002387 -0.000497

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XY XZ YZ

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1 Atom -0.007021 -0.000752 -0.000640

2 Atom -0.001278 0.006532 0.007996

3 Atom 0.002556 0.004323 0.009922

4 Atom 0.002757 -0.001134 -0.000752

5 Atom 0.000626 0.003101 0.003544

6 Atom 0.000000 0.000000 -0.003594

7 Atom -0.002556 -0.004323 0.009922

8 Atom 0.001278 -0.006532 0.007996

9 Atom 0.007021 0.000752 -0.000640

10 Atom -0.000626 -0.003101 0.003544

11 Atom -0.002757 0.001134 -0.000752

12 Atom 0.000000 0.017095 0.000000

13 Atom -0.000626 0.003101 -0.003544

14 Atom -0.002757 -0.001134 0.000752

15 Atom -0.002556 0.004323 -0.009922

16 Atom 0.001278 0.006532 -0.007996

17 Atom 0.007021 -0.000752 0.000640

18 Atom 0.000000 0.000000 0.003594

19 Atom -0.001278 -0.006532 -0.007996

20 Atom 0.002556 -0.004323 -0.009922

21 Atom 0.002757 0.001134 0.000752

22 Atom 0.000626 -0.003101 -0.003544

23 Atom -0.007021 0.000752 0.000640

24 Atom 0.000000 -0.017095 0.000000

25 Atom 0.000000 0.000000 0.000000

26 Atom -0.002150 -0.000957 0.000869

27 Atom -0.001102 0.001746 -0.001561

28 Atom -0.000040 -0.000576 0.000617

29 Atom -0.000851 0.001187 -0.001313

30 Atom 0.002150 0.000957 0.000869

31 Atom 0.001102 -0.001746 -0.001561

32 Atom 0.000040 0.000576 0.000617

33 Atom 0.000851 -0.001187 -0.001313

34 Atom -0.000851 -0.001187 0.001313

35 Atom -0.000040 0.000576 -0.000617

36 Atom -0.001102 -0.001746 0.001561

37 Atom -0.002150 0.000957 -0.000869

38 Atom 0.002150 -0.000957 -0.000869

39 Atom 0.001102 0.001746 0.001561

40 Atom 0.000040 -0.000576 -0.000617

41 Atom 0.000851 0.001187 0.001313

42 Atom -0.002085 -0.000103 0.000092

43 Atom 0.001529 0.000036 0.000038

44 Atom 0.002085 0.000103 0.000092

45 Atom -0.001529 -0.000036 0.000038

46 Atom 0.001529 -0.000036 -0.000038

47 Atom -0.002085 0.000103 -0.000092

48 Atom 0.002085 -0.000103 -0.000092

49 Atom -0.001529 0.000036 -0.000038

50 Atom -0.000211 0.000045 -0.000015

51 Atom -0.002217 0.000140 -0.000015

52 Atom 0.000211 -0.000045 -0.000015

53 Atom 0.002217 -0.000140 -0.000015

54 Atom -0.002217 -0.000140 0.000015

55 Atom -0.000211 -0.000045 0.000015

56 Atom 0.000211 0.000045 0.000015

57 Atom 0.002217 0.000140 0.000015

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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 -0.0213 -2.856 -1.019 -0.953 0.0312 0.0252 0.9992

1 C(13) Bbb 0.0033 0.446 0.159 0.149 0.8026 0.5951 -0.0401

Bcc 0.0180 2.410 0.860 0.804 -0.5957 0.8032 -0.0017

Baa -0.0379 -1.461 -0.521 -0.487 0.5730 0.8141 -0.0941

2 N(14) Bbb -0.0341 -1.317 -0.470 -0.439 0.8174 -0.5761 -0.0070

Bcc 0.0720 2.778 0.991 0.926 0.0599 0.0730 0.9955

Baa -0.0972 -13.045 -4.655 -4.351 -0.6943 0.7195 -0.0144

3 C(13) Bbb -0.0924 -12.399 -4.424 -4.136 0.7195 0.6936 -0.0355

Bcc 0.1896 25.444 9.079 8.487 0.0155 0.0350 0.9993

Baa -0.0144 -1.938 -0.692 -0.646 0.0497 0.0279 0.9984

4 C(13) Bbb 0.0044 0.591 0.211 0.197 0.7531 -0.6577 -0.0191

Bcc 0.0100 1.347 0.481 0.449 0.6561 0.7528 -0.0537

Baa -0.0281 -3.769 -1.345 -1.257 -0.6646 0.7472 -0.0071

5 C(13) Bbb -0.0271 -3.636 -1.298 -1.213 0.7462 0.6632 -0.0569

Bcc 0.0552 7.406 2.643 2.470 0.0378 0.0431 0.9984

Baa -0.1086 -4.190 -1.495 -1.398 0.0000 0.0231 0.9997

6 N(14) Bbb 0.0470 1.811 0.646 0.604 0.0000 0.9997 -0.0231

Bcc 0.0617 2.379 0.849 0.793 1.0000 0.0000 0.0000

Baa -0.0972 -13.045 -4.655 -4.351 0.6943 0.7195 -0.0144

7 C(13) Bbb -0.0924 -12.399 -4.424 -4.136 0.7195 -0.6936 0.0355

Bcc 0.1896 25.444 9.079 8.487 -0.0155 0.0350 0.9993

Baa -0.0379 -1.461 -0.521 -0.487 -0.5730 0.8141 -0.0941

8 N(14) Bbb -0.0341 -1.317 -0.470 -0.439 0.8174 0.5761 0.0070

Bcc 0.0720 2.778 0.991 0.926 -0.0599 0.0730 0.9955

Baa -0.0213 -2.856 -1.019 -0.953 -0.0312 0.0252 0.9992

9 C(13) Bbb 0.0033 0.446 0.159 0.149 0.8026 -0.5951 0.0401

Bcc 0.0180 2.410 0.860 0.804 0.5957 0.8032 -0.0017

Baa -0.0281 -3.769 -1.345 -1.257 0.6646 0.7472 -0.0071

10 C(13) Bbb -0.0271 -3.636 -1.298 -1.213 0.7462 -0.6632 0.0569

Bcc 0.0552 7.406 2.643 2.470 -0.0378 0.0431 0.9984

Baa -0.0144 -1.938 -0.692 -0.646 -0.0497 0.0279 0.9984

11 C(13) Bbb 0.0044 0.591 0.211 0.197 0.7531 0.6577 0.0191

Bcc 0.0100 1.347 0.481 0.449 -0.6561 0.7528 -0.0537

Baa -0.1888 -7.283 -2.599 -2.429 0.0000 1.0000 0.0000

12 N(14) Bbb -0.1877 -7.240 -2.583 -2.415 0.9995 0.0000 -0.0303

Bcc 0.3765 14.522 5.182 4.844 0.0303 0.0000 0.9995

Baa -0.0281 -3.769 -1.345 -1.257 0.6646 0.7472 0.0071

13 C(13) Bbb -0.0271 -3.636 -1.298 -1.213 0.7462 -0.6632 -0.0569

Bcc 0.0552 7.406 2.643 2.470 0.0378 -0.0431 0.9984

Baa -0.0144 -1.938 -0.692 -0.646 0.0497 -0.0279 0.9984

14 C(13) Bbb 0.0044 0.591 0.211 0.197 0.7531 0.6577 -0.0191

Bcc 0.0100 1.347 0.481 0.449 -0.6561 0.7528 0.0537

Baa -0.0972 -13.045 -4.655 -4.351 0.6943 0.7195 0.0144

15 C(13) Bbb -0.0924 -12.399 -4.424 -4.136 0.7195 -0.6936 -0.0355

Bcc 0.1896 25.444 9.079 8.487 0.0155 -0.0350 0.9993

Baa -0.0379 -1.461 -0.521 -0.487 -0.5730 0.8141 0.0941

16 N(14) Bbb -0.0341 -1.317 -0.470 -0.439 0.8174 0.5761 -0.0070

Bcc 0.0720 2.778 0.991 0.926 0.0599 -0.0730 0.9955

Baa -0.0213 -2.856 -1.019 -0.953 0.0312 -0.0252 0.9992

17 C(13) Bbb 0.0033 0.446 0.159 0.149 0.8026 -0.5951 -0.0401

Bcc 0.0180 2.410 0.860 0.804 0.5957 0.8032 0.0017

Baa -0.1086 -4.190 -1.495 -1.398 0.0000 -0.0231 0.9997

18 N(14) Bbb 0.0470 1.811 0.646 0.604 0.0000 0.9997 0.0231

Bcc 0.0617 2.379 0.849 0.793 1.0000 0.0000 0.0000

Baa -0.0379 -1.461 -0.521 -0.487 0.5730 0.8141 0.0941

19 N(14) Bbb -0.0341 -1.317 -0.470 -0.439 0.8174 -0.5761 0.0070

Bcc 0.0720 2.778 0.991 0.926 -0.0599 -0.0730 0.9955

Baa -0.0972 -13.045 -4.655 -4.351 -0.6943 0.7195 0.0144

20 C(13) Bbb -0.0924 -12.399 -4.424 -4.136 0.7195 0.6936 0.0355

Bcc 0.1896 25.444 9.079 8.487 -0.0155 -0.0350 0.9993

Baa -0.0144 -1.938 -0.692 -0.646 -0.0497 -0.0279 0.9984

21 C(13) Bbb 0.0044 0.591 0.211 0.197 0.7531 -0.6577 0.0191

Bcc 0.0100 1.347 0.481 0.449 0.6561 0.7528 0.0537

Baa -0.0281 -3.769 -1.345 -1.257 -0.6646 0.7472 0.0071

22 C(13) Bbb -0.0271 -3.636 -1.298 -1.213 0.7462 0.6632 0.0569

Bcc 0.0552 7.406 2.643 2.470 -0.0378 -0.0431 0.9984

Baa -0.0213 -2.856 -1.019 -0.953 -0.0312 -0.0252 0.9992

23 C(13) Bbb 0.0033 0.446 0.159 0.149 0.8026 0.5951 0.0401

Bcc 0.0180 2.410 0.860 0.804 -0.5957 0.8032 0.0017

Baa -0.1888 -7.283 -2.599 -2.429 0.0000 1.0000 0.0000

24 N(14) Bbb -0.1877 -7.240 -2.583 -2.415 0.9995 0.0000 0.0303

Bcc 0.3765 14.522 5.182 4.844 -0.0303 0.0000 0.9995

Baa -0.0069 -0.231 -0.083 -0.077 0.0000 1.0000 0.0000

25 Zn(67) Bbb 0.0012 0.041 0.015 0.014 0.0000 0.0000 1.0000

Bcc 0.0057 0.191 0.068 0.064 1.0000 0.0000 0.0000

Baa -0.0224 -3.009 -1.074 -1.004 0.0268 -0.0242 0.9993

26 C(13) Bbb 0.0090 1.212 0.433 0.404 0.6875 0.7261 -0.0009

Bcc 0.0134 1.796 0.641 0.599 0.7256 -0.6871 -0.0361

Baa -0.0248 -3.328 -1.187 -1.110 0.4291 0.9032 0.0092

27 C(13) Bbb -0.0221 -2.960 -1.056 -0.987 0.9029 -0.4286 -0.0326

Bcc 0.0469 6.287 2.244 2.097 0.0255 -0.0223 0.9994

Baa -0.0166 -2.233 -0.797 -0.745 0.0225 -0.0253 0.9994

28 C(13) Bbb 0.0077 1.030 0.368 0.344 0.0424 0.9988 0.0244

Bcc 0.0090 1.203 0.429 0.401 0.9988 -0.0418 -0.0235

Baa -0.0180 -2.416 -0.862 -0.806 0.8515 0.5243 -0.0062

29 C(13) Bbb -0.0162 -2.169 -0.774 -0.724 -0.5238 0.8511 0.0346

Bcc 0.0342 4.585 1.636 1.529 0.0234 -0.0262 0.9994

Baa -0.0224 -3.009 -1.074 -1.004 -0.0268 -0.0242 0.9993

30 C(13) Bbb 0.0090 1.212 0.433 0.404 -0.6875 0.7261 -0.0009

Bcc 0.0134 1.796 0.641 0.599 0.7256 0.6871 0.0361

Baa -0.0248 -3.328 -1.187 -1.110 -0.4291 0.9032 0.0092

31 C(13) Bbb -0.0221 -2.960 -1.056 -0.987 0.9029 0.4286 0.0326

Bcc 0.0469 6.287 2.244 2.097 -0.0255 -0.0223 0.9994

Baa -0.0166 -2.233 -0.797 -0.745 -0.0225 -0.0253 0.9994

32 C(13) Bbb 0.0077 1.030 0.368 0.344 -0.0424 0.9988 0.0244

Bcc 0.0090 1.203 0.429 0.401 0.9988 0.0418 0.0235

Baa -0.0180 -2.416 -0.862 -0.806 0.8515 -0.5243 0.0062

33 C(13) Bbb -0.0162 -2.169 -0.774 -0.724 0.5238 0.8511 0.0346

Bcc 0.0342 4.585 1.636 1.529 -0.0234 -0.0262 0.9994

Baa -0.0180 -2.416 -0.862 -0.806 0.8515 0.5243 0.0062

34 C(13) Bbb -0.0162 -2.169 -0.774 -0.724 -0.5238 0.8511 -0.0346

Bcc 0.0342 4.585 1.636 1.529 -0.0234 0.0262 0.9994

Baa -0.0166 -2.233 -0.797 -0.745 -0.0225 0.0253 0.9994

35 C(13) Bbb 0.0077 1.030 0.368 0.344 0.0424 0.9988 -0.0244

Bcc 0.0090 1.203 0.429 0.401 0.9988 -0.0418 0.0235

Baa -0.0248 -3.328 -1.187 -1.110 0.4291 0.9032 -0.0092

36 C(13) Bbb -0.0221 -2.960 -1.056 -0.987 0.9029 -0.4286 0.0326

Bcc 0.0469 6.287 2.244 2.097 -0.0255 0.0223 0.9994

Baa -0.0224 -3.009 -1.074 -1.004 -0.0268 0.0242 0.9993

37 C(13) Bbb 0.0090 1.212 0.433 0.404 0.6875 0.7261 0.0009

Bcc 0.0134 1.796 0.641 0.599 0.7256 -0.6871 0.0361

Baa -0.0224 -3.009 -1.074 -1.004 0.0268 0.0242 0.9993

38 C(13) Bbb 0.0090 1.212 0.433 0.404 -0.6875 0.7261 0.0009

Bcc 0.0134 1.796 0.641 0.599 0.7256 0.6871 -0.0361

Baa -0.0248 -3.328 -1.187 -1.110 -0.4291 0.9032 -0.0092

39 C(13) Bbb -0.0221 -2.960 -1.056 -0.987 0.9029 0.4286 -0.0326

Bcc 0.0469 6.287 2.244 2.097 0.0255 0.0223 0.9994

Baa -0.0166 -2.233 -0.797 -0.745 0.0225 0.0253 0.9994

40 C(13) Bbb 0.0077 1.030 0.368 0.344 -0.0424 0.9988 -0.0244

Bcc 0.0090 1.203 0.429 0.401 0.9988 0.0418 -0.0235

Baa -0.0180 -2.416 -0.862 -0.806 0.8515 -0.5243 -0.0062

41 C(13) Bbb -0.0162 -2.169 -0.774 -0.724 0.5238 0.8511 -0.0346

Bcc 0.0342 4.585 1.636 1.529 0.0234 0.0262 0.9994

Baa -0.0015 -0.815 -0.291 -0.272 0.0104 -0.0362 0.9993

42 H(1) Bbb -0.0014 -0.723 -0.258 -0.241 0.6444 0.7644 0.0210

Bcc 0.0029 1.538 0.549 0.513 0.7646 -0.6437 -0.0313

Baa -0.0012 -0.644 -0.230 -0.215 -0.0918 0.0403 0.9950

43 H(1) Bbb -0.0011 -0.586 -0.209 -0.196 0.8435 -0.5279 0.0992

Bcc 0.0023 1.230 0.439 0.410 0.5293 0.8483 0.0145

Baa -0.0015 -0.815 -0.291 -0.272 -0.0104 -0.0362 0.9993

44 H(1) Bbb -0.0014 -0.723 -0.258 -0.241 -0.6444 0.7644 0.0210

Bcc 0.0029 1.538 0.549 0.513 0.7646 0.6437 0.0313

Baa -0.0012 -0.644 -0.230 -0.215 0.0918 0.0403 0.9950

45 H(1) Bbb -0.0011 -0.586 -0.209 -0.196 0.8435 0.5279 -0.0992

Bcc 0.0023 1.230 0.439 0.410 -0.5293 0.8483 0.0145

Baa -0.0012 -0.644 -0.230 -0.215 0.0918 -0.0403 0.9950

46 H(1) Bbb -0.0011 -0.586 -0.209 -0.196 0.8435 -0.5279 -0.0992

Bcc 0.0023 1.230 0.439 0.410 0.5293 0.8483 -0.0145

Baa -0.0015 -0.815 -0.291 -0.272 -0.0104 0.0362 0.9993

47 H(1) Bbb -0.0014 -0.723 -0.258 -0.241 0.6444 0.7644 -0.0210

Bcc 0.0029 1.538 0.549 0.513 0.7646 -0.6437 0.0313

Baa -0.0015 -0.815 -0.291 -0.272 0.0104 0.0362 0.9993

48 H(1) Bbb -0.0014 -0.723 -0.258 -0.241 -0.6444 0.7644 -0.0210

Bcc 0.0029 1.538 0.549 0.513 0.7646 0.6437 -0.0313

Baa -0.0012 -0.644 -0.230 -0.215 -0.0918 -0.0403 0.9950

49 H(1) Bbb -0.0011 -0.586 -0.209 -0.196 0.8435 0.5279 0.0992

Bcc 0.0023 1.230 0.439 0.410 -0.5293 0.8483 -0.0145

Baa -0.0008 -0.423 -0.151 -0.141 -0.0238 0.0158 0.9996

50 H(1) Bbb -0.0002 -0.110 -0.039 -0.037 0.1785 0.9839 -0.0113

Bcc 0.0010 0.533 0.190 0.178 0.9837 -0.1781 0.0262

Baa -0.0032 -1.705 -0.608 -0.569 0.3429 0.9393 -0.0126

51 H(1) Bbb -0.0005 -0.267 -0.095 -0.089 -0.0262 0.0230 0.9994

Bcc 0.0037 1.972 0.704 0.658 0.9390 -0.3423 0.0325

Baa -0.0008 -0.423 -0.151 -0.141 0.0238 0.0158 0.9996

52 H(1) Bbb -0.0002 -0.110 -0.039 -0.037 -0.1785 0.9839 -0.0113

Bcc 0.0010 0.533 0.190 0.178 0.9837 0.1781 -0.0262

Baa -0.0032 -1.705 -0.608 -0.569 -0.3429 0.9393 -0.0126

53 H(1) Bbb -0.0005 -0.267 -0.095 -0.089 0.0262 0.0230 0.9994

Bcc 0.0037 1.972 0.704 0.658 0.9390 0.3423 -0.0325

Baa -0.0032 -1.705 -0.608 -0.569 0.3429 0.9393 0.0126

54 H(1) Bbb -0.0005 -0.267 -0.095 -0.089 0.0262 -0.0230 0.9994

Bcc 0.0037 1.972 0.704 0.658 0.9390 -0.3423 -0.0325

Baa -0.0008 -0.423 -0.151 -0.141 0.0238 -0.0158 0.9996

55 H(1) Bbb -0.0002 -0.110 -0.039 -0.037 0.1785 0.9839 0.0113

Bcc 0.0010 0.533 0.190 0.178 0.9837 -0.1781 -0.0262

Baa -0.0008 -0.423 -0.151 -0.141 -0.0238 -0.0158 0.9996

56 H(1) Bbb -0.0002 -0.110 -0.039 -0.037 -0.1785 0.9839 0.0113

Bcc 0.0010 0.533 0.190 0.178 0.9837 0.1781 0.0262

Baa -0.0032 -1.705 -0.608 -0.569 -0.3429 0.9393 0.0126

57 H(1) Bbb -0.0005 -0.267 -0.095 -0.089 -0.0262 -0.0230 0.9994

Bcc 0.0037 1.972 0.704 0.658 0.9390 0.3423 0.0325

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

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Sat Jun 15 12:23:07 2019, MaxMem= 1342177280 cpu: 42.0

(Enter /apps/gaussian/g09d01/g09/l9999.exe)

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9\0\\#p opt b3lyp/genecp scrf=(solvent=dmso,smd) empiricaldispersion=g

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668666,-2.8089711611,-0.080976616\C,-5.1631867793,-4.1574510341,-0.124

2541901\C,-4.1696829056,-5.1549166378,-0.1242096179\C,-2.8185079821,-4

.8268339125,-0.0806103493\C,-2.8185079821,4.8268339125,-0.0806103493\C

,-4.1696829056,5.1549166378,-0.1242096179\C,-5.1631867793,4.1574510341

,-0.1242541901\C,-4.8198668666,2.8089711611,-0.080976616\C,4.819866866

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2\H,-2.0569105681,-5.5997393601,-0.0833458549\H,-2.0569105681,5.599739

3601,-0.0833458549\H,-5.5831231335,2.037691608,-0.0837838532\H,5.58312

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471853,4.4470873137,-0.1595734526\H,6.2081471853,-4.4470873137,-0.1595

734526\H,4.4665680054,-6.1981532853,-0.1595145842\H,-4.4665680054,-6.1

981532853,-0.1595145842\H,-6.2081471853,-4.4470873137,-0.1595734526\\V

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upole=-3.9793274,-1.7876403,5.7669677,0.,0.,0.\PG=C02V [C2(Zn1),SGV(N2

),SGV'(N2),X(C32H16N4)]\\@

Experience is what you get when you don't get what you want.

-- Dan Stanford

Job cpu time: 0 days 3 hours 23 minutes 2.9 seconds.

File lengths (MBytes): RWF= 1379 Int= 0 D2E= 0 Chk= 62 Scr= 2

Normal termination of Gaussian 09 at Sat Jun 15 12:23:08 2019.