Entering Gaussian System, Link 0=g09

Input=TPPcation.com

Output=TPPcation.log

Initial command:

/home/kira/g09/l1.exe "/home/kira/g09/scratch/Gau-13637.inp" -scrdir="/home/kira/g09/scratch/"

Entering Link 1 = /home/kira/g09/l1.exe PID= 13644.

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Cite this work as:

Gaussian 09, Revision E.01,

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

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

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

Gaussian 09: ES64L-G09RevE.01 30-Nov-2015

18-Aug-2019

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

%nprocshared=8

Will use up to 8 processors via shared memory.

%mem=15GB

%chk=TPPcation.chk

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

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

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

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

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

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

4//1;

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

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

7//1,2,3,16;

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

2/9=110/2;

99//99;

2/9=110/2;

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

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

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

7//1,2,3,16;

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

2/9=110/2;

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

99/9=1/99;

Leave Link 1 at Sun Aug 18 13:41:05 2019, MaxMem= 2013265920 cpu: 0.5

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

---------

TPPcation

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Symbolic Z-matrix:

Charge = 1 Multiplicity = 2

C -0.68416 4.23797 0.1734

C -1.13173 2.88312 0.0404

N 0. 2.10277 -0.02395

C 1.13173 2.88312 0.0404

C 0.68416 4.23797 0.1734

C 2.45874 2.43876 -0.00975

C 2.8605 1.09096 -0.06504

N 2.0397 0. 0.00961

C 2.8605 -1.09096 -0.06504

C 4.24999 -0.67741 -0.22258

C 4.24999 0.67741 -0.22258

C -2.45874 2.43876 -0.00975

C -2.8605 1.09096 -0.06504

C -4.24999 0.67741 -0.22258

C -4.24999 -0.67741 -0.22258

C -2.8605 -1.09096 -0.06504

N -2.0397 0. 0.00961

C -2.45874 -2.43876 -0.00975

C -1.13173 -2.88312 0.0404

C -0.68416 -4.23797 0.1734

C 0.68416 -4.23797 0.1734

C 1.13173 -2.88312 0.0404

N 0. -2.10277 -0.02395

C 2.45874 -2.43876 -0.00975

C 3.51916 3.48937 0.00178

C 3.63978 4.39529 -1.05869

C 4.63245 5.37237 -1.04642

C 5.51516 5.4605 0.02908

C 5.40114 4.56435 1.09112

C 4.41154 3.58452 1.07644

C -5.51516 5.4605 0.02908

C -4.63245 5.37237 -1.04642

C -3.63978 4.39529 -1.05869

C -3.51916 3.48937 0.00178

C -4.41154 3.58452 1.07644

C -5.40114 4.56435 1.09112

C 3.51916 -3.48937 0.00178

C 4.41154 -3.58452 1.07644

C 5.40114 -4.56435 1.09112

C 5.51516 -5.4605 0.02908

C 4.63245 -5.37237 -1.04642

C 3.63978 -4.39529 -1.05869

C -3.51916 -3.48937 0.00178

C -4.41154 -3.58452 1.07644

C -5.40114 -4.56435 1.09112

C -5.51516 -5.4605 0.02908

C -4.63245 -5.37237 -1.04642

C -3.63978 -4.39529 -1.05869

H -1.33286 5.0936 0.26959

H 1.33286 5.0936 0.26959

H 5.09797 -1.33486 -0.33683

H 5.09797 1.33486 -0.33683

H -5.09797 1.33486 -0.33683

H -5.09797 -1.33486 -0.33683

H -1.33286 -5.0936 0.26959

H 1.33286 -5.0936 0.26959

H 2.95811 4.32551 -1.89933

H 4.71729 6.06291 -1.87896

H 6.28725 6.22262 0.03949

H 6.08164 4.62858 1.93371

H 4.32232 2.89106 1.90541

H -6.28725 6.22262 0.03949

H -4.71729 6.06291 -1.87896

H -2.95811 4.32551 -1.89933

H -4.32232 2.89106 1.90541

H -6.08164 4.62858 1.93371

H 4.32232 -2.89106 1.90541

H 6.08164 -4.62858 1.93371

H 6.28725 -6.22262 0.03949

H 4.71729 -6.06291 -1.87896

H 2.95811 -4.32551 -1.89933

H -4.32232 -2.89106 1.90541

H -6.08164 -4.62858 1.93371

H -6.28725 -6.22262 0.03949

H -4.71729 -6.06291 -1.87896

H -2.95811 -4.32551 -1.89933

H 0. 1.09244 -0.08272

H 0. -1.09244 -0.08272

NAtoms= 78 NQM= 78 NQMF= 0 NMMI= 0 NMMIF= 0

NMic= 0 NMicF= 0.

Isotopes and Nuclear Properties:

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

in nuclear magnetons)

Atom 1 2 3 4 5 6 7 8 9 10

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

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

NucSpn= 0 0 2 0 0 0 0 2 0 0

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

NQMom= 0.0000000 0.0000000 2.0440000 0.0000000 0.0000000 0.0000000 0.0000000 2.0440000 0.0000000 0.0000000

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

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

Atom 11 12 13 14 15 16 17 18 19 20

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

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

NucSpn= 0 0 0 0 0 0 2 0 0 0

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

NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 2.0440000 0.0000000 0.0000000 0.0000000

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

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

Atom 21 22 23 24 25 26 27 28 29 30

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

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

NucSpn= 0 0 2 0 0 0 0 0 0 0

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

NQMom= 0.0000000 0.0000000 2.0440000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

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

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

Atom 31 32 33 34 35 36 37 38 39 40

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

AtmWgt= 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000

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

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

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

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

AtZNuc= 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000

Atom 41 42 43 44 45 46 47 48 49 50

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

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

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

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

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

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

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

Atom 51 52 53 54 55 56 57 58 59 60

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

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

NucSpn= 1 1 1 1 1 1 1 1 1 1

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

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

NMagM= 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460

AtZNuc= 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000

Atom 61 62 63 64 65 66 67 68 69 70

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

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

NucSpn= 1 1 1 1 1 1 1 1 1 1

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

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

NMagM= 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460

AtZNuc= 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000

Atom 71 72 73 74 75 76 77 78

IAtWgt= 1 1 1 1 1 1 1 1

AtmWgt= 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250

NucSpn= 1 1 1 1 1 1 1 1

AtZEff= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NMagM= 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460

AtZNuc= 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000

Leave Link 101 at Sun Aug 18 13:41:05 2019, MaxMem= 2013265920 cpu: 3.3

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Initialization pass.

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

! Initial Parameters !

! (Angstroms and Degrees) !

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

! Name Definition Value Derivative Info. !

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

! R1 R(1,2) 1.433 estimate D2E/DX2 !

! R2 R(1,5) 1.3683 estimate D2E/DX2 !

! R3 R(1,49) 1.078 estimate D2E/DX2 !

! R4 R(2,3) 1.3762 estimate D2E/DX2 !

! R5 R(2,12) 1.4003 estimate D2E/DX2 !

! R6 R(3,4) 1.3762 estimate D2E/DX2 !

! R7 R(3,77) 1.012 estimate D2E/DX2 !

! R8 R(4,5) 1.433 estimate D2E/DX2 !

! R9 R(4,6) 1.4003 estimate D2E/DX2 !

! R10 R(5,50) 1.078 estimate D2E/DX2 !

! R11 R(6,7) 1.4075 estimate D2E/DX2 !

! R12 R(6,25) 1.4928 estimate D2E/DX2 !

! R13 R(7,8) 1.3673 estimate D2E/DX2 !

! R14 R(7,11) 1.4583 estimate D2E/DX2 !

! R15 R(8,9) 1.3673 estimate D2E/DX2 !

! R16 R(9,10) 1.4583 estimate D2E/DX2 !

! R17 R(9,24) 1.4075 estimate D2E/DX2 !

! R18 R(10,11) 1.3548 estimate D2E/DX2 !

! R19 R(10,51) 1.0791 estimate D2E/DX2 !

! R20 R(11,52) 1.0791 estimate D2E/DX2 !

! R21 R(12,13) 1.4075 estimate D2E/DX2 !

! R22 R(12,34) 1.4928 estimate D2E/DX2 !

! R23 R(13,14) 1.4583 estimate D2E/DX2 !

! R24 R(13,17) 1.3673 estimate D2E/DX2 !

! R25 R(14,15) 1.3548 estimate D2E/DX2 !

! R26 R(14,53) 1.0791 estimate D2E/DX2 !

! R27 R(15,16) 1.4583 estimate D2E/DX2 !

! R28 R(15,54) 1.0791 estimate D2E/DX2 !

! R29 R(16,17) 1.3673 estimate D2E/DX2 !

! R30 R(16,18) 1.4075 estimate D2E/DX2 !

! R31 R(18,19) 1.4003 estimate D2E/DX2 !

! R32 R(18,43) 1.4928 estimate D2E/DX2 !

! R33 R(19,20) 1.433 estimate D2E/DX2 !

! R34 R(19,23) 1.3762 estimate D2E/DX2 !

! R35 R(20,21) 1.3683 estimate D2E/DX2 !

! R36 R(20,55) 1.078 estimate D2E/DX2 !

! R37 R(21,22) 1.433 estimate D2E/DX2 !

! R38 R(21,56) 1.078 estimate D2E/DX2 !

! R39 R(22,23) 1.3762 estimate D2E/DX2 !

! R40 R(22,24) 1.4003 estimate D2E/DX2 !

! R41 R(23,78) 1.012 estimate D2E/DX2 !

! R42 R(24,37) 1.4928 estimate D2E/DX2 !

! R43 R(25,26) 1.3999 estimate D2E/DX2 !

! R44 R(25,30) 1.4001 estimate D2E/DX2 !

! R45 R(26,27) 1.3929 estimate D2E/DX2 !

! R46 R(26,57) 1.0845 estimate D2E/DX2 !

! R47 R(27,28) 1.3942 estimate D2E/DX2 !

! R48 R(27,58) 1.085 estimate D2E/DX2 !

! R49 R(28,29) 1.3943 estimate D2E/DX2 !

! R50 R(28,59) 1.0849 estimate D2E/DX2 !

! R51 R(29,30) 1.3927 estimate D2E/DX2 !

! R52 R(29,60) 1.085 estimate D2E/DX2 !

! R53 R(30,61) 1.0845 estimate D2E/DX2 !

! R54 R(31,32) 1.3942 estimate D2E/DX2 !

! R55 R(31,36) 1.3943 estimate D2E/DX2 !

! R56 R(31,62) 1.0849 estimate D2E/DX2 !

! R57 R(32,33) 1.3929 estimate D2E/DX2 !

! R58 R(32,63) 1.085 estimate D2E/DX2 !

! R59 R(33,34) 1.3999 estimate D2E/DX2 !

! R60 R(33,64) 1.0845 estimate D2E/DX2 !

! R61 R(34,35) 1.4001 estimate D2E/DX2 !

! R62 R(35,36) 1.3927 estimate D2E/DX2 !

! R63 R(35,65) 1.0845 estimate D2E/DX2 !

! R64 R(36,66) 1.085 estimate D2E/DX2 !

! R65 R(37,38) 1.4001 estimate D2E/DX2 !

! R66 R(37,42) 1.3999 estimate D2E/DX2 !

! R67 R(38,39) 1.3927 estimate D2E/DX2 !

! R68 R(38,67) 1.0845 estimate D2E/DX2 !

! R69 R(39,40) 1.3943 estimate D2E/DX2 !

! R70 R(39,68) 1.085 estimate D2E/DX2 !

! R71 R(40,41) 1.3942 estimate D2E/DX2 !

! R72 R(40,69) 1.0849 estimate D2E/DX2 !

! R73 R(41,42) 1.3929 estimate D2E/DX2 !

! R74 R(41,70) 1.085 estimate D2E/DX2 !

! R75 R(42,71) 1.0845 estimate D2E/DX2 !

! R76 R(43,44) 1.4001 estimate D2E/DX2 !

! R77 R(43,48) 1.3999 estimate D2E/DX2 !

! R78 R(44,45) 1.3927 estimate D2E/DX2 !

! R79 R(44,72) 1.0845 estimate D2E/DX2 !

! R80 R(45,46) 1.3943 estimate D2E/DX2 !

! R81 R(45,73) 1.085 estimate D2E/DX2 !

! R82 R(46,47) 1.3942 estimate D2E/DX2 !

! R83 R(46,74) 1.0849 estimate D2E/DX2 !

! R84 R(47,48) 1.3929 estimate D2E/DX2 !

! R85 R(47,75) 1.085 estimate D2E/DX2 !

! R86 R(48,76) 1.0845 estimate D2E/DX2 !

! A1 A(2,1,5) 108.1992 estimate D2E/DX2 !

! A2 A(2,1,49) 124.8005 estimate D2E/DX2 !

! A3 A(5,1,49) 126.9951 estimate D2E/DX2 !

! A4 A(1,2,3) 106.4747 estimate D2E/DX2 !

! A5 A(1,2,12) 126.8202 estimate D2E/DX2 !

! A6 A(3,2,12) 126.7047 estimate D2E/DX2 !

! A7 A(2,3,4) 110.6443 estimate D2E/DX2 !

! A8 A(2,3,77) 124.6662 estimate D2E/DX2 !

! A9 A(4,3,77) 124.6662 estimate D2E/DX2 !

! A10 A(3,4,5) 106.4747 estimate D2E/DX2 !

! A11 A(3,4,6) 126.7047 estimate D2E/DX2 !

! A12 A(5,4,6) 126.8202 estimate D2E/DX2 !

! A13 A(1,5,4) 108.1992 estimate D2E/DX2 !

! A14 A(1,5,50) 126.9951 estimate D2E/DX2 !

! A15 A(4,5,50) 124.8005 estimate D2E/DX2 !

! A16 A(4,6,7) 125.1543 estimate D2E/DX2 !

! A17 A(4,6,25) 116.7153 estimate D2E/DX2 !

! A18 A(7,6,25) 118.13 estimate D2E/DX2 !

! A19 A(6,7,8) 126.1965 estimate D2E/DX2 !

! A20 A(6,7,11) 123.2159 estimate D2E/DX2 !

! A21 A(8,7,11) 110.5866 estimate D2E/DX2 !

! A22 A(7,8,9) 105.8598 estimate D2E/DX2 !

! A23 A(8,9,10) 110.5866 estimate D2E/DX2 !

! A24 A(8,9,24) 126.1965 estimate D2E/DX2 !

! A25 A(10,9,24) 123.2159 estimate D2E/DX2 !

! A26 A(9,10,11) 106.4747 estimate D2E/DX2 !

! A27 A(9,10,51) 125.9756 estimate D2E/DX2 !

! A28 A(11,10,51) 127.5377 estimate D2E/DX2 !

! A29 A(7,11,10) 106.4747 estimate D2E/DX2 !

! A30 A(7,11,52) 125.9756 estimate D2E/DX2 !

! A31 A(10,11,52) 127.5377 estimate D2E/DX2 !

! A32 A(2,12,13) 125.1543 estimate D2E/DX2 !

! A33 A(2,12,34) 116.7153 estimate D2E/DX2 !

! A34 A(13,12,34) 118.13 estimate D2E/DX2 !

! A35 A(12,13,14) 123.2159 estimate D2E/DX2 !

! A36 A(12,13,17) 126.1965 estimate D2E/DX2 !

! A37 A(14,13,17) 110.5866 estimate D2E/DX2 !

! A38 A(13,14,15) 106.4747 estimate D2E/DX2 !

! A39 A(13,14,53) 125.9756 estimate D2E/DX2 !

! A40 A(15,14,53) 127.5377 estimate D2E/DX2 !

! A41 A(14,15,16) 106.4747 estimate D2E/DX2 !

! A42 A(14,15,54) 127.5377 estimate D2E/DX2 !

! A43 A(16,15,54) 125.9756 estimate D2E/DX2 !

! A44 A(15,16,17) 110.5866 estimate D2E/DX2 !

! A45 A(15,16,18) 123.2159 estimate D2E/DX2 !

! A46 A(17,16,18) 126.1965 estimate D2E/DX2 !

! A47 A(13,17,16) 105.8598 estimate D2E/DX2 !

! A48 A(16,18,19) 125.1543 estimate D2E/DX2 !

! A49 A(16,18,43) 118.13 estimate D2E/DX2 !

! A50 A(19,18,43) 116.7153 estimate D2E/DX2 !

! A51 A(18,19,20) 126.8202 estimate D2E/DX2 !

! A52 A(18,19,23) 126.7047 estimate D2E/DX2 !

! A53 A(20,19,23) 106.4747 estimate D2E/DX2 !

! A54 A(19,20,21) 108.1992 estimate D2E/DX2 !

! A55 A(19,20,55) 124.8005 estimate D2E/DX2 !

! A56 A(21,20,55) 126.9951 estimate D2E/DX2 !

! A57 A(20,21,22) 108.1992 estimate D2E/DX2 !

! A58 A(20,21,56) 126.9951 estimate D2E/DX2 !

! A59 A(22,21,56) 124.8005 estimate D2E/DX2 !

! A60 A(21,22,23) 106.4747 estimate D2E/DX2 !

! A61 A(21,22,24) 126.8202 estimate D2E/DX2 !

! A62 A(23,22,24) 126.7047 estimate D2E/DX2 !

! A63 A(19,23,22) 110.6443 estimate D2E/DX2 !

! A64 A(19,23,78) 124.6662 estimate D2E/DX2 !

! A65 A(22,23,78) 124.6662 estimate D2E/DX2 !

! A66 A(9,24,22) 125.1543 estimate D2E/DX2 !

! A67 A(9,24,37) 118.13 estimate D2E/DX2 !

! A68 A(22,24,37) 116.7153 estimate D2E/DX2 !

! A69 A(6,25,26) 120.7166 estimate D2E/DX2 !

! A70 A(6,25,30) 120.4324 estimate D2E/DX2 !

! A71 A(26,25,30) 118.851 estimate D2E/DX2 !

! A72 A(25,26,27) 120.5745 estimate D2E/DX2 !

! A73 A(25,26,57) 119.4304 estimate D2E/DX2 !

! A74 A(27,26,57) 119.9924 estimate D2E/DX2 !

! A75 A(26,27,28) 120.1559 estimate D2E/DX2 !

! A76 A(26,27,58) 119.6979 estimate D2E/DX2 !

! A77 A(28,27,58) 120.146 estimate D2E/DX2 !

! A78 A(27,28,29) 119.6834 estimate D2E/DX2 !

! A79 A(27,28,59) 120.1585 estimate D2E/DX2 !

! A80 A(29,28,59) 120.1581 estimate D2E/DX2 !

! A81 A(28,29,30) 120.1507 estimate D2E/DX2 !

! A82 A(28,29,60) 120.1458 estimate D2E/DX2 !

! A83 A(30,29,60) 119.7033 estimate D2E/DX2 !

! A84 A(25,30,29) 120.5839 estimate D2E/DX2 !

! A85 A(25,30,61) 119.3952 estimate D2E/DX2 !

! A86 A(29,30,61) 120.0194 estimate D2E/DX2 !

! A87 A(32,31,36) 119.6834 estimate D2E/DX2 !

! A88 A(32,31,62) 120.1585 estimate D2E/DX2 !

! A89 A(36,31,62) 120.1581 estimate D2E/DX2 !

! A90 A(31,32,33) 120.1559 estimate D2E/DX2 !

! A91 A(31,32,63) 120.146 estimate D2E/DX2 !

! A92 A(33,32,63) 119.6979 estimate D2E/DX2 !

! A93 A(32,33,34) 120.5745 estimate D2E/DX2 !

! A94 A(32,33,64) 119.9924 estimate D2E/DX2 !

! A95 A(34,33,64) 119.4304 estimate D2E/DX2 !

! A96 A(12,34,33) 120.7166 estimate D2E/DX2 !

! A97 A(12,34,35) 120.4324 estimate D2E/DX2 !

! A98 A(33,34,35) 118.851 estimate D2E/DX2 !

! A99 A(34,35,36) 120.5839 estimate D2E/DX2 !

! A100 A(34,35,65) 119.3952 estimate D2E/DX2 !

! A101 A(36,35,65) 120.0194 estimate D2E/DX2 !

! A102 A(31,36,35) 120.1507 estimate D2E/DX2 !

! A103 A(31,36,66) 120.1458 estimate D2E/DX2 !

! A104 A(35,36,66) 119.7033 estimate D2E/DX2 !

! A105 A(24,37,38) 120.4324 estimate D2E/DX2 !

! A106 A(24,37,42) 120.7166 estimate D2E/DX2 !

! A107 A(38,37,42) 118.851 estimate D2E/DX2 !

! A108 A(37,38,39) 120.5839 estimate D2E/DX2 !

! A109 A(37,38,67) 119.3952 estimate D2E/DX2 !

! A110 A(39,38,67) 120.0194 estimate D2E/DX2 !

! A111 A(38,39,40) 120.1507 estimate D2E/DX2 !

! A112 A(38,39,68) 119.7033 estimate D2E/DX2 !

! A113 A(40,39,68) 120.1458 estimate D2E/DX2 !

! A114 A(39,40,41) 119.6834 estimate D2E/DX2 !

! A115 A(39,40,69) 120.1581 estimate D2E/DX2 !

! A116 A(41,40,69) 120.1585 estimate D2E/DX2 !

! A117 A(40,41,42) 120.1559 estimate D2E/DX2 !

! A118 A(40,41,70) 120.146 estimate D2E/DX2 !

! A119 A(42,41,70) 119.6979 estimate D2E/DX2 !

! A120 A(37,42,41) 120.5745 estimate D2E/DX2 !

! A121 A(37,42,71) 119.4304 estimate D2E/DX2 !

! A122 A(41,42,71) 119.9924 estimate D2E/DX2 !

! A123 A(18,43,44) 120.4324 estimate D2E/DX2 !

! A124 A(18,43,48) 120.7166 estimate D2E/DX2 !

! A125 A(44,43,48) 118.851 estimate D2E/DX2 !

! A126 A(43,44,45) 120.5839 estimate D2E/DX2 !

! A127 A(43,44,72) 119.3952 estimate D2E/DX2 !

! A128 A(45,44,72) 120.0194 estimate D2E/DX2 !

! A129 A(44,45,46) 120.1507 estimate D2E/DX2 !

! A130 A(44,45,73) 119.7033 estimate D2E/DX2 !

! A131 A(46,45,73) 120.1458 estimate D2E/DX2 !

! A132 A(45,46,47) 119.6834 estimate D2E/DX2 !

! A133 A(45,46,74) 120.1581 estimate D2E/DX2 !

! A134 A(47,46,74) 120.1585 estimate D2E/DX2 !

! A135 A(46,47,48) 120.1559 estimate D2E/DX2 !

! A136 A(46,47,75) 120.146 estimate D2E/DX2 !

! A137 A(48,47,75) 119.6979 estimate D2E/DX2 !

! A138 A(43,48,47) 120.5745 estimate D2E/DX2 !

! A139 A(43,48,76) 119.4304 estimate D2E/DX2 !

! A140 A(47,48,76) 119.9924 estimate D2E/DX2 !

! D1 D(5,1,2,3) 0.5297 estimate D2E/DX2 !

! D2 D(5,1,2,12) -179.6684 estimate D2E/DX2 !

! D3 D(49,1,2,3) -178.6847 estimate D2E/DX2 !

! D4 D(49,1,2,12) 1.1172 estimate D2E/DX2 !

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

! D6 D(2,1,5,50) -179.1923 estimate D2E/DX2 !

! D7 D(49,1,5,4) 179.1923 estimate D2E/DX2 !

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

! D9 D(1,2,3,4) -0.8845 estimate D2E/DX2 !

! D10 D(1,2,3,77) 177.4318 estimate D2E/DX2 !

! D11 D(12,2,3,4) 179.3133 estimate D2E/DX2 !

! D12 D(12,2,3,77) -2.3705 estimate D2E/DX2 !

! D13 D(1,2,12,13) -176.1919 estimate D2E/DX2 !

! D14 D(1,2,12,34) 3.5881 estimate D2E/DX2 !

! D15 D(3,2,12,13) 3.5712 estimate D2E/DX2 !

! D16 D(3,2,12,34) -176.6488 estimate D2E/DX2 !

! D17 D(2,3,4,5) 0.8845 estimate D2E/DX2 !

! D18 D(2,3,4,6) -179.3133 estimate D2E/DX2 !

! D19 D(77,3,4,5) -177.4318 estimate D2E/DX2 !

! D20 D(77,3,4,6) 2.3705 estimate D2E/DX2 !

! D21 D(3,4,5,1) -0.5297 estimate D2E/DX2 !

! D22 D(3,4,5,50) 178.6847 estimate D2E/DX2 !

! D23 D(6,4,5,1) 179.6684 estimate D2E/DX2 !

! D24 D(6,4,5,50) -1.1172 estimate D2E/DX2 !

! D25 D(3,4,6,7) -3.5712 estimate D2E/DX2 !

! D26 D(3,4,6,25) 176.6488 estimate D2E/DX2 !

! D27 D(5,4,6,7) 176.1919 estimate D2E/DX2 !

! D28 D(5,4,6,25) -3.5881 estimate D2E/DX2 !

! D29 D(4,6,7,8) -4.6109 estimate D2E/DX2 !

! D30 D(4,6,7,11) 174.985 estimate D2E/DX2 !

! D31 D(25,6,7,8) 175.1663 estimate D2E/DX2 !

! D32 D(25,6,7,11) -5.2378 estimate D2E/DX2 !

! D33 D(4,6,25,26) -64.8626 estimate D2E/DX2 !

! D34 D(4,6,25,30) 115.1427 estimate D2E/DX2 !

! D35 D(7,6,25,26) 115.3413 estimate D2E/DX2 !

! D36 D(7,6,25,30) -64.6533 estimate D2E/DX2 !

! D37 D(6,7,8,9) -179.0579 estimate D2E/DX2 !

! D38 D(11,7,8,9) 1.3032 estimate D2E/DX2 !

! D39 D(6,7,11,10) 179.5292 estimate D2E/DX2 !

! D40 D(6,7,11,52) -1.6515 estimate D2E/DX2 !

! D41 D(8,7,11,10) -0.8192 estimate D2E/DX2 !

! D42 D(8,7,11,52) 178.0001 estimate D2E/DX2 !

! D43 D(7,8,9,10) -1.3032 estimate D2E/DX2 !

! D44 D(7,8,9,24) 179.0579 estimate D2E/DX2 !

! D45 D(8,9,10,11) 0.8192 estimate D2E/DX2 !

! D46 D(8,9,10,51) -178.0001 estimate D2E/DX2 !

! D47 D(24,9,10,11) -179.5292 estimate D2E/DX2 !

! D48 D(24,9,10,51) 1.6515 estimate D2E/DX2 !

! D49 D(8,9,24,22) 4.6109 estimate D2E/DX2 !

! D50 D(8,9,24,37) -175.1663 estimate D2E/DX2 !

! D51 D(10,9,24,22) -174.985 estimate D2E/DX2 !

! D52 D(10,9,24,37) 5.2378 estimate D2E/DX2 !

! D53 D(9,10,11,7) 0.0 estimate D2E/DX2 !

! D54 D(9,10,11,52) -178.795 estimate D2E/DX2 !

! D55 D(51,10,11,7) 178.795 estimate D2E/DX2 !

! D56 D(51,10,11,52) 0.0 estimate D2E/DX2 !

! D57 D(2,12,13,14) -174.985 estimate D2E/DX2 !

! D58 D(2,12,13,17) 4.6109 estimate D2E/DX2 !

! D59 D(34,12,13,14) 5.2378 estimate D2E/DX2 !

! D60 D(34,12,13,17) -175.1663 estimate D2E/DX2 !

! D61 D(2,12,34,33) 64.8626 estimate D2E/DX2 !

! D62 D(2,12,34,35) -115.1427 estimate D2E/DX2 !

! D63 D(13,12,34,33) -115.3413 estimate D2E/DX2 !

! D64 D(13,12,34,35) 64.6533 estimate D2E/DX2 !

! D65 D(12,13,14,15) -179.5292 estimate D2E/DX2 !

! D66 D(12,13,14,53) 1.6515 estimate D2E/DX2 !

! D67 D(17,13,14,15) 0.8192 estimate D2E/DX2 !

! D68 D(17,13,14,53) -178.0001 estimate D2E/DX2 !

! D69 D(12,13,17,16) 179.0579 estimate D2E/DX2 !

! D70 D(14,13,17,16) -1.3032 estimate D2E/DX2 !

! D71 D(13,14,15,16) 0.0 estimate D2E/DX2 !

! D72 D(13,14,15,54) -178.795 estimate D2E/DX2 !

! D73 D(53,14,15,16) 178.795 estimate D2E/DX2 !

! D74 D(53,14,15,54) 0.0 estimate D2E/DX2 !

! D75 D(14,15,16,17) -0.8192 estimate D2E/DX2 !

! D76 D(14,15,16,18) 179.5292 estimate D2E/DX2 !

! D77 D(54,15,16,17) 178.0001 estimate D2E/DX2 !

! D78 D(54,15,16,18) -1.6515 estimate D2E/DX2 !

! D79 D(15,16,17,13) 1.3032 estimate D2E/DX2 !

! D80 D(18,16,17,13) -179.0579 estimate D2E/DX2 !

! D81 D(15,16,18,19) 174.985 estimate D2E/DX2 !

! D82 D(15,16,18,43) -5.2378 estimate D2E/DX2 !

! D83 D(17,16,18,19) -4.6109 estimate D2E/DX2 !

! D84 D(17,16,18,43) 175.1663 estimate D2E/DX2 !

! D85 D(16,18,19,20) 176.1919 estimate D2E/DX2 !

! D86 D(16,18,19,23) -3.5712 estimate D2E/DX2 !

! D87 D(43,18,19,20) -3.5881 estimate D2E/DX2 !

! D88 D(43,18,19,23) 176.6488 estimate D2E/DX2 !

! D89 D(16,18,43,44) -64.6533 estimate D2E/DX2 !

! D90 D(16,18,43,48) 115.3413 estimate D2E/DX2 !

! D91 D(19,18,43,44) 115.1427 estimate D2E/DX2 !

! D92 D(19,18,43,48) -64.8626 estimate D2E/DX2 !

! D93 D(18,19,20,21) 179.6684 estimate D2E/DX2 !

! D94 D(18,19,20,55) -1.1172 estimate D2E/DX2 !

! D95 D(23,19,20,21) -0.5297 estimate D2E/DX2 !

! D96 D(23,19,20,55) 178.6847 estimate D2E/DX2 !

! D97 D(18,19,23,22) -179.3133 estimate D2E/DX2 !

! D98 D(18,19,23,78) 2.3705 estimate D2E/DX2 !

! D99 D(20,19,23,22) 0.8845 estimate D2E/DX2 !

! D100 D(20,19,23,78) -177.4318 estimate D2E/DX2 !

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

! D102 D(19,20,21,56) 179.1923 estimate D2E/DX2 !

! D103 D(55,20,21,22) -179.1923 estimate D2E/DX2 !

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

! D105 D(20,21,22,23) 0.5297 estimate D2E/DX2 !

! D106 D(20,21,22,24) -179.6684 estimate D2E/DX2 !

! D107 D(56,21,22,23) -178.6847 estimate D2E/DX2 !

! D108 D(56,21,22,24) 1.1172 estimate D2E/DX2 !

! D109 D(21,22,23,19) -0.8845 estimate D2E/DX2 !

! D110 D(21,22,23,78) 177.4318 estimate D2E/DX2 !

! D111 D(24,22,23,19) 179.3133 estimate D2E/DX2 !

! D112 D(24,22,23,78) -2.3705 estimate D2E/DX2 !

! D113 D(21,22,24,9) -176.1919 estimate D2E/DX2 !

! D114 D(21,22,24,37) 3.5881 estimate D2E/DX2 !

! D115 D(23,22,24,9) 3.5712 estimate D2E/DX2 !

! D116 D(23,22,24,37) -176.6488 estimate D2E/DX2 !

! D117 D(9,24,37,38) 64.6533 estimate D2E/DX2 !

! D118 D(9,24,37,42) -115.3413 estimate D2E/DX2 !

! D119 D(22,24,37,38) -115.1427 estimate D2E/DX2 !

! D120 D(22,24,37,42) 64.8626 estimate D2E/DX2 !

! D121 D(6,25,26,27) -179.8409 estimate D2E/DX2 !

! D122 D(6,25,26,57) -0.4402 estimate D2E/DX2 !

! D123 D(30,25,26,27) 0.1538 estimate D2E/DX2 !

! D124 D(30,25,26,57) 179.5545 estimate D2E/DX2 !

! D125 D(6,25,30,29) -179.9309 estimate D2E/DX2 !

! D126 D(6,25,30,61) -0.3723 estimate D2E/DX2 !

! D127 D(26,25,30,29) 0.0744 estimate D2E/DX2 !

! D128 D(26,25,30,61) 179.633 estimate D2E/DX2 !

! D129 D(25,26,27,28) -0.2524 estimate D2E/DX2 !

! D130 D(25,26,27,58) 179.5845 estimate D2E/DX2 !

! D131 D(57,26,27,28) -179.6497 estimate D2E/DX2 !

! D132 D(57,26,27,58) 0.1871 estimate D2E/DX2 !

! D133 D(26,27,28,29) 0.1206 estimate D2E/DX2 !

! D134 D(26,27,28,59) -179.8926 estimate D2E/DX2 !

! D135 D(58,27,28,29) -179.7154 estimate D2E/DX2 !

! D136 D(58,27,28,59) 0.2713 estimate D2E/DX2 !

! D137 D(27,28,29,30) 0.1066 estimate D2E/DX2 !

! D138 D(27,28,29,60) -179.7629 estimate D2E/DX2 !

! D139 D(59,28,29,30) -179.8802 estimate D2E/DX2 !

! D140 D(59,28,29,60) 0.2503 estimate D2E/DX2 !

! D141 D(28,29,30,25) -0.2049 estimate D2E/DX2 !

! D142 D(28,29,30,61) -179.7608 estimate D2E/DX2 !

! D143 D(60,29,30,25) 179.6652 estimate D2E/DX2 !

! D144 D(60,29,30,61) 0.1093 estimate D2E/DX2 !

! D145 D(36,31,32,33) -0.1206 estimate D2E/DX2 !

! D146 D(36,31,32,63) 179.7154 estimate D2E/DX2 !

! D147 D(62,31,32,33) 179.8926 estimate D2E/DX2 !

! D148 D(62,31,32,63) -0.2713 estimate D2E/DX2 !

! D149 D(32,31,36,35) -0.1066 estimate D2E/DX2 !

! D150 D(32,31,36,66) 179.7629 estimate D2E/DX2 !

! D151 D(62,31,36,35) 179.8802 estimate D2E/DX2 !

! D152 D(62,31,36,66) -0.2503 estimate D2E/DX2 !

! D153 D(31,32,33,34) 0.2524 estimate D2E/DX2 !

! D154 D(31,32,33,64) 179.6497 estimate D2E/DX2 !

! D155 D(63,32,33,34) -179.5845 estimate D2E/DX2 !

! D156 D(63,32,33,64) -0.1871 estimate D2E/DX2 !

! D157 D(32,33,34,12) 179.8409 estimate D2E/DX2 !

! D158 D(32,33,34,35) -0.1538 estimate D2E/DX2 !

! D159 D(64,33,34,12) 0.4402 estimate D2E/DX2 !

! D160 D(64,33,34,35) -179.5545 estimate D2E/DX2 !

! D161 D(12,34,35,36) 179.9309 estimate D2E/DX2 !

! D162 D(12,34,35,65) 0.3723 estimate D2E/DX2 !

! D163 D(33,34,35,36) -0.0744 estimate D2E/DX2 !

! D164 D(33,34,35,65) -179.633 estimate D2E/DX2 !

! D165 D(34,35,36,31) 0.2049 estimate D2E/DX2 !

! D166 D(34,35,36,66) -179.6652 estimate D2E/DX2 !

! D167 D(65,35,36,31) 179.7608 estimate D2E/DX2 !

! D168 D(65,35,36,66) -0.1093 estimate D2E/DX2 !

! D169 D(24,37,38,39) 179.9309 estimate D2E/DX2 !

! D170 D(24,37,38,67) 0.3723 estimate D2E/DX2 !

! D171 D(42,37,38,39) -0.0744 estimate D2E/DX2 !

! D172 D(42,37,38,67) -179.633 estimate D2E/DX2 !

! D173 D(24,37,42,41) 179.8409 estimate D2E/DX2 !

! D174 D(24,37,42,71) 0.4402 estimate D2E/DX2 !

! D175 D(38,37,42,41) -0.1538 estimate D2E/DX2 !

! D176 D(38,37,42,71) -179.5545 estimate D2E/DX2 !

! D177 D(37,38,39,40) 0.2049 estimate D2E/DX2 !

! D178 D(37,38,39,68) -179.6652 estimate D2E/DX2 !

! D179 D(67,38,39,40) 179.7608 estimate D2E/DX2 !

! D180 D(67,38,39,68) -0.1093 estimate D2E/DX2 !

! D181 D(38,39,40,41) -0.1066 estimate D2E/DX2 !

! D182 D(38,39,40,69) 179.8802 estimate D2E/DX2 !

! D183 D(68,39,40,41) 179.7629 estimate D2E/DX2 !

! D184 D(68,39,40,69) -0.2503 estimate D2E/DX2 !

! D185 D(39,40,41,42) -0.1206 estimate D2E/DX2 !

! D186 D(39,40,41,70) 179.7154 estimate D2E/DX2 !

! D187 D(69,40,41,42) 179.8926 estimate D2E/DX2 !

! D188 D(69,40,41,70) -0.2713 estimate D2E/DX2 !

! D189 D(40,41,42,37) 0.2524 estimate D2E/DX2 !

! D190 D(40,41,42,71) 179.6497 estimate D2E/DX2 !

! D191 D(70,41,42,37) -179.5845 estimate D2E/DX2 !

! D192 D(70,41,42,71) -0.1871 estimate D2E/DX2 !

! D193 D(18,43,44,45) -179.9309 estimate D2E/DX2 !

! D194 D(18,43,44,72) -0.3723 estimate D2E/DX2 !

! D195 D(48,43,44,45) 0.0744 estimate D2E/DX2 !

! D196 D(48,43,44,72) 179.633 estimate D2E/DX2 !

! D197 D(18,43,48,47) -179.8409 estimate D2E/DX2 !

! D198 D(18,43,48,76) -0.4402 estimate D2E/DX2 !

! D199 D(44,43,48,47) 0.1538 estimate D2E/DX2 !

! D200 D(44,43,48,76) 179.5545 estimate D2E/DX2 !

! D201 D(43,44,45,46) -0.2049 estimate D2E/DX2 !

! D202 D(43,44,45,73) 179.6652 estimate D2E/DX2 !

! D203 D(72,44,45,46) -179.7608 estimate D2E/DX2 !

! D204 D(72,44,45,73) 0.1093 estimate D2E/DX2 !

! D205 D(44,45,46,47) 0.1066 estimate D2E/DX2 !

! D206 D(44,45,46,74) -179.8802 estimate D2E/DX2 !

! D207 D(73,45,46,47) -179.7629 estimate D2E/DX2 !

! D208 D(73,45,46,74) 0.2503 estimate D2E/DX2 !

! D209 D(45,46,47,48) 0.1206 estimate D2E/DX2 !

! D210 D(45,46,47,75) -179.7154 estimate D2E/DX2 !

! D211 D(74,46,47,48) -179.8926 estimate D2E/DX2 !

! D212 D(74,46,47,75) 0.2713 estimate D2E/DX2 !

! D213 D(46,47,48,43) -0.2524 estimate D2E/DX2 !

! D214 D(46,47,48,76) -179.6497 estimate D2E/DX2 !

! D215 D(75,47,48,43) 179.5845 estimate D2E/DX2 !

! D216 D(75,47,48,76) 0.1871 estimate D2E/DX2 !

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

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

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Aug 18 13:41:05 2019, MaxMem= 2013265920 cpu: 0.1

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

Stoichiometry C44H30N4(1+,2)

Framework group C2V[SGV(H2N2),SGV'(N2),X(C44H28)]

Deg. of freedom 59

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 -0.684157 4.237971 0.173400

2 6 0 -1.131729 2.883123 0.040396

3 7 0 0.000000 2.102773 -0.023951

4 6 0 1.131729 2.883123 0.040396

5 6 0 0.684157 4.237971 0.173400

6 6 0 2.458736 2.438755 -0.009747

7 6 0 2.860501 1.090959 -0.065036

8 7 0 2.039697 -0.000000 0.009609

9 6 0 2.860501 -1.090959 -0.065036

10 6 0 4.249993 -0.677406 -0.222575

11 6 0 4.249993 0.677406 -0.222575

12 6 0 -2.458736 2.438755 -0.009747

13 6 0 -2.860501 1.090959 -0.065036

14 6 0 -4.249993 0.677406 -0.222575

15 6 0 -4.249993 -0.677406 -0.222575

16 6 0 -2.860501 -1.090959 -0.065036

17 7 0 -2.039697 0.000000 0.009609

18 6 0 -2.458736 -2.438755 -0.009747

19 6 0 -1.131729 -2.883123 0.040396

20 6 0 -0.684157 -4.237971 0.173400

21 6 0 0.684157 -4.237971 0.173400

22 6 0 1.131729 -2.883123 0.040396

23 7 0 -0.000000 -2.102773 -0.023951

24 6 0 2.458736 -2.438755 -0.009747

25 6 0 3.519159 3.489365 0.001777

26 6 0 3.639775 4.395294 -1.058689

27 6 0 4.632445 5.372370 -1.046425

28 6 0 5.515158 5.460502 0.029084

29 6 0 5.401135 4.564352 1.091122

30 6 0 4.411543 3.584521 1.076438

31 6 0 -5.515158 5.460502 0.029084

32 6 0 -4.632445 5.372370 -1.046425

33 6 0 -3.639775 4.395294 -1.058689

34 6 0 -3.519159 3.489365 0.001777

35 6 0 -4.411543 3.584521 1.076438

36 6 0 -5.401135 4.564352 1.091122

37 6 0 3.519159 -3.489365 0.001777

38 6 0 4.411543 -3.584521 1.076438

39 6 0 5.401135 -4.564352 1.091122

40 6 0 5.515158 -5.460502 0.029084

41 6 0 4.632445 -5.372370 -1.046425

42 6 0 3.639775 -4.395294 -1.058689

43 6 0 -3.519159 -3.489365 0.001777

44 6 0 -4.411543 -3.584521 1.076438

45 6 0 -5.401135 -4.564352 1.091122

46 6 0 -5.515158 -5.460502 0.029084

47 6 0 -4.632445 -5.372370 -1.046425

48 6 0 -3.639775 -4.395294 -1.058689

49 1 0 -1.332862 5.093596 0.269591

50 1 0 1.332862 5.093596 0.269591

51 1 0 5.097972 -1.334858 -0.336827

52 1 0 5.097972 1.334858 -0.336827

53 1 0 -5.097972 1.334858 -0.336827

54 1 0 -5.097972 -1.334858 -0.336827

55 1 0 -1.332862 -5.093596 0.269591

56 1 0 1.332862 -5.093596 0.269591

57 1 0 2.958110 4.325512 -1.899332

58 1 0 4.717290 6.062914 -1.878958

59 1 0 6.287254 6.222625 0.039493

60 1 0 6.081643 4.628576 1.933705

61 1 0 4.322318 2.891059 1.905414

62 1 0 -6.287254 6.222625 0.039493

63 1 0 -4.717290 6.062914 -1.878958

64 1 0 -2.958110 4.325512 -1.899332

65 1 0 -4.322318 2.891059 1.905414

66 1 0 -6.081643 4.628576 1.933705

67 1 0 4.322318 -2.891059 1.905414

68 1 0 6.081643 -4.628576 1.933705

69 1 0 6.287254 -6.222625 0.039493

70 1 0 4.717290 -6.062914 -1.878958

71 1 0 2.958110 -4.325512 -1.899332

72 1 0 -4.322318 -2.891059 1.905414

73 1 0 -6.081643 -4.628576 1.933705

74 1 0 -6.287254 -6.222625 0.039493

75 1 0 -4.717290 -6.062914 -1.878958

76 1 0 -2.958110 -4.325512 -1.899332

77 1 0 0.000000 1.092438 -0.082721

78 1 0 -0.000000 -1.092438 -0.082721

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

Rotational constants (GHZ): 0.0588256 0.0580329 0.0301998

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

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

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

There are 261 symmetry adapted cartesian basis functions of A1 symmetry.

There are 240 symmetry adapted cartesian basis functions of A2 symmetry.

There are 249 symmetry adapted cartesian basis functions of B1 symmetry.

There are 252 symmetry adapted cartesian basis functions of B2 symmetry.

There are 248 symmetry adapted basis functions of A1 symmetry.

There are 229 symmetry adapted basis functions of A2 symmetry.

There are 237 symmetry adapted basis functions of B1 symmetry.

There are 240 symmetry adapted basis functions of B2 symmetry.

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

161 alpha electrons 160 beta electrons

nuclear repulsion energy 5359.0290093584 Hartrees.

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

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

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

NAtoms= 78 NActive= 78 NUniq= 21 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=T Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2121186179 Hartrees.

Nuclear repulsion after empirical dispersion term = 5358.8168907404 Hartrees.

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Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 78

GePol: Total number of spheres = 78

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

GePol: Number of points = 5698

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.11D-07

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 294

GePol: Fraction of low-weight points (<1% of avg) = 5.16%

GePol: Cavity surface area = 616.128 Ang\*\*2

GePol: Cavity volume = 627.764 Ang\*\*3

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

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

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PCM non-electrostatic energy = -0.0020588737 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5358.8148318668 Hartrees.

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(Enter /home/kira/g09/l302.exe)

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

NBasis= 954 RedAO= T EigKep= 6.24D-05 NBF= 248 229 237 240

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 248 229 237 240

Precomputing XC quadrature grid using

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

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

NSgBfM= 939 939 939 939 940 MxSgAt= 78 MxSgA2= 78.

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

DipDrv: MaxL=1.

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

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -1914.09039253798

JPrj=0 DoOrth=F DoCkMO=F.

Initial guess orbital symmetries:

Alpha Orbitals:

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

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Beta Orbitals:

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

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The electronic state of the initial guess is 2-A1.

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

Leave Link 401 at Sun Aug 18 13:41:09 2019, MaxMem= 2013265920 cpu: 18.1

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3049894 IEndB= 3049894 NGot= 2013265920 MDV= 2011237673

LenX= 2011237673 LenY= 2010232667

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

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

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

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

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

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 97401612.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.33D-15 for 5687.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.11D-15 for 3427 3156.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.33D-15 for 5687.

Iteration 1 A^-1\*A deviation from orthogonality is 3.01D-12 for 4406 4396.

E= -1913.30831337962

DIIS: error= 4.79D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1913.30831337962 IErMin= 1 ErrMin= 4.79D-02

ErrMax= 4.79D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.80D+00 BMatP= 3.80D+00

IDIUse=3 WtCom= 5.21D-01 WtEn= 4.79D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.114 Goal= None Shift= 0.000

Gap= 0.031 Goal= None Shift= 0.000

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

Damping current iteration by 2.50D-01

RMSDP=1.81D-03 MaxDP=9.78D-02 OVMax= 2.84D-01

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.48D-04 CP: 9.91D-01

E= -1913.61912326370 Delta-E= -0.310809884078 Rises=F Damp=T

DIIS: error= 2.66D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1913.61912326370 IErMin= 2 ErrMin= 2.66D-02

ErrMax= 2.66D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.22D+00 BMatP= 3.80D+00

IDIUse=3 WtCom= 7.34D-01 WtEn= 2.66D-01

Coeff-Com: -0.108D+01 0.208D+01

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

Coeff: -0.793D+00 0.179D+01

Gap= 0.122 Goal= None Shift= 0.000

Gap= 0.073 Goal= None Shift= 0.000

RMSDP=6.70D-04 MaxDP=3.35D-02 DE=-3.11D-01 OVMax= 2.29D-01

Cycle 3 Pass 1 IDiag 1:

RMSU= 4.66D-04 CP: 9.77D-01 2.06D+00

E= -1914.17170659246 Delta-E= -0.552583328754 Rises=F Damp=F

DIIS: error= 5.95D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.17170659246 IErMin= 3 ErrMin= 5.95D-03

ErrMax= 5.95D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.01D-01 BMatP= 1.22D+00

IDIUse=3 WtCom= 9.40D-01 WtEn= 5.95D-02

Coeff-Com: -0.360D+00 0.713D+00 0.647D+00

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

Coeff: -0.339D+00 0.670D+00 0.668D+00

Gap= 0.103 Goal= None Shift= 0.000

Gap= 0.040 Goal= None Shift= 0.000

RMSDP=2.49D-04 MaxDP=1.86D-02 DE=-5.53D-01 OVMax= 5.87D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.81D-04 CP: 9.82D-01 2.02D+00 6.39D-01

E= -1914.18960146250 Delta-E= -0.017894870042 Rises=F Damp=F

DIIS: error= 3.63D-03 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.18960146250 IErMin= 4 ErrMin= 3.63D-03

ErrMax= 3.63D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.28D-02 BMatP= 1.01D-01

IDIUse=3 WtCom= 9.64D-01 WtEn= 3.63D-02

Coeff-Com: -0.614D-01 0.129D+00 0.373D+00 0.560D+00

Coeff-En: 0.000D+00 0.000D+00 0.243D+00 0.757D+00

Coeff: -0.591D-01 0.124D+00 0.368D+00 0.567D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.048 Goal= None Shift= 0.000

RMSDP=1.11D-04 MaxDP=6.84D-03 DE=-1.79D-02 OVMax= 2.93D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 7.32D-05 CP: 9.80D-01 2.01D+00 7.05D-01 5.83D-01

E= -1914.19743856923 Delta-E= -0.007837106735 Rises=F Damp=F

DIIS: error= 1.47D-03 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.19743856923 IErMin= 5 ErrMin= 1.47D-03

ErrMax= 1.47D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.32D-03 BMatP= 3.28D-02

IDIUse=3 WtCom= 9.85D-01 WtEn= 1.47D-02

Coeff-Com: -0.625D-02 0.145D-01 0.151D+00 0.321D+00 0.520D+00

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

Coeff: -0.615D-02 0.142D-01 0.149D+00 0.316D+00 0.527D+00

Gap= 0.103 Goal= None Shift= 0.000

Gap= 0.048 Goal= None Shift= 0.000

RMSDP=4.12D-05 MaxDP=3.07D-03 DE=-7.84D-03 OVMax= 1.58D-02

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.29D-05 CP: 9.80D-01 2.02D+00 7.32D-01 6.33D-01 5.88D-01

E= -1914.19821563208 Delta-E= -0.000777062849 Rises=F Damp=F

DIIS: error= 5.57D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.19821563208 IErMin= 6 ErrMin= 5.57D-04

ErrMax= 5.57D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.93D-04 BMatP= 3.32D-03

IDIUse=3 WtCom= 9.94D-01 WtEn= 5.57D-03

Coeff-Com: 0.109D-02-0.197D-02 0.489D-01 0.127D+00 0.307D+00 0.519D+00

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

Coeff: 0.108D-02-0.196D-02 0.486D-01 0.126D+00 0.305D+00 0.521D+00

Gap= 0.103 Goal= None Shift= 0.000

Gap= 0.049 Goal= None Shift= 0.000

RMSDP=1.40D-05 MaxDP=1.32D-03 DE=-7.77D-04 OVMax= 3.53D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 9.68D-06 CP: 9.80D-01 2.01D+00 7.30D-01 6.34D-01 6.93D-01

CP: 7.44D-01

E= -1914.19832336337 Delta-E= -0.000107731291 Rises=F Damp=F

DIIS: error= 2.39D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.19832336337 IErMin= 7 ErrMin= 2.39D-04

ErrMax= 2.39D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.92D-05 BMatP= 3.93D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.39D-03

Coeff-Com: 0.145D-02-0.336D-02 0.170D-03 0.141D-01 0.806D-01 0.275D+00

Coeff-Com: 0.632D+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: 0.145D-02-0.335D-02 0.170D-03 0.141D-01 0.804D-01 0.275D+00

Coeff: 0.633D+00

Gap= 0.102 Goal= None Shift= 0.000

Gap= 0.050 Goal= None Shift= 0.000

RMSDP=6.52D-06 MaxDP=6.66D-04 DE=-1.08D-04 OVMax= 2.95D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 5.07D-06 CP: 9.80D-01 2.02D+00 7.31D-01 6.44D-01 6.93D-01

CP: 8.89D-01 9.04D-01

E= -1914.19835347867 Delta-E= -0.000030115300 Rises=F Damp=F

DIIS: error= 1.46D-04 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.19835347867 IErMin= 8 ErrMin= 1.46D-04

ErrMax= 1.46D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.54D-05 BMatP= 5.92D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.46D-03

Coeff-Com: 0.970D-04-0.407D-03-0.242D-01-0.569D-01-0.117D+00-0.162D+00

Coeff-Com: 0.257D+00 0.110D+01

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

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

Coeff: 0.969D-04-0.407D-03-0.242D-01-0.568D-01-0.117D+00-0.162D+00

Coeff: 0.256D+00 0.110D+01

Gap= 0.102 Goal= None Shift= 0.000

Gap= 0.050 Goal= None Shift= 0.000

RMSDP=6.49D-06 MaxDP=6.29D-04 DE=-3.01D-05 OVMax= 2.81D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.16D-06 CP: 9.80D-01 2.02D+00 7.31D-01 6.47D-01 7.29D-01

CP: 1.01D+00 1.34D+00 1.44D+00

E= -1914.19837103898 Delta-E= -0.000017560309 Rises=F Damp=F

DIIS: error= 7.32D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.19837103898 IErMin= 9 ErrMin= 7.32D-05

ErrMax= 7.32D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.19D-06 BMatP= 1.54D-05

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

Coeff-Com: -0.327D-03 0.540D-03-0.130D-01-0.335D-01-0.777D-01-0.138D+00

Coeff-Com: 0.288D-01 0.581D+00 0.653D+00

Coeff: -0.327D-03 0.540D-03-0.130D-01-0.335D-01-0.777D-01-0.138D+00

Coeff: 0.288D-01 0.581D+00 0.653D+00

Gap= 0.101 Goal= None Shift= 0.000

Gap= 0.051 Goal= None Shift= 0.000

RMSDP=2.07D-06 MaxDP=2.03D-04 DE=-1.76D-05 OVMax= 8.54D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 9.80D-07 CP: 9.80D-01 2.02D+00 7.31D-01 6.48D-01 7.32D-01

CP: 1.05D+00 1.45D+00 1.65D+00 9.47D-01

E= -1914.19837326552 Delta-E= -0.000002226537 Rises=F Damp=F

DIIS: error= 3.05D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.19837326552 IErMin=10 ErrMin= 3.05D-05

ErrMax= 3.05D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.15D-07 BMatP= 4.19D-06

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

Coeff-Com: -0.187D-03 0.365D-03 0.450D-04-0.155D-02-0.636D-02-0.230D-01

Coeff-Com: -0.433D-01-0.195D-01 0.313D+00 0.781D+00

Coeff: -0.187D-03 0.365D-03 0.450D-04-0.155D-02-0.636D-02-0.230D-01

Coeff: -0.433D-01-0.195D-01 0.313D+00 0.781D+00

Gap= 0.101 Goal= None Shift= 0.000

Gap= 0.051 Goal= None Shift= 0.000

RMSDP=8.37D-07 MaxDP=8.50D-05 DE=-2.23D-06 OVMax= 3.51D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 4.12D-07 CP: 9.80D-01 2.02D+00 7.31D-01 6.48D-01 7.34D-01

CP: 1.06D+00 1.49D+00 1.73D+00 1.10D+00 9.30D-01

E= -1914.19837359730 Delta-E= -0.000000331785 Rises=F Damp=F

DIIS: error= 7.16D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.19837359730 IErMin=11 ErrMin= 7.16D-06

ErrMax= 7.16D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.26D-08 BMatP= 7.15D-07

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

Coeff-Com: -0.563D-04 0.115D-03 0.870D-03 0.150D-02 0.227D-02-0.207D-02

Coeff-Com: -0.201D-01-0.507D-01 0.106D+00 0.369D+00 0.593D+00

Coeff: -0.563D-04 0.115D-03 0.870D-03 0.150D-02 0.227D-02-0.207D-02

Coeff: -0.201D-01-0.507D-01 0.106D+00 0.369D+00 0.593D+00

Gap= 0.101 Goal= None Shift= 0.000

Gap= 0.051 Goal= None Shift= 0.000

RMSDP=2.23D-07 MaxDP=1.72D-05 DE=-3.32D-07 OVMax= 8.93D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.78D-07 CP: 9.80D-01 2.02D+00 7.31D-01 6.48D-01 7.34D-01

CP: 1.06D+00 1.49D+00 1.73D+00 1.14D+00 1.01D+00

CP: 1.01D+00

E= -1914.19837363621 Delta-E= -0.000000038908 Rises=F Damp=F

DIIS: error= 5.44D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.19837363621 IErMin=12 ErrMin= 5.44D-06

ErrMax= 5.44D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.44D-08 BMatP= 9.26D-08

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

Coeff-Com: 0.488D-04-0.858D-04 0.375D-03 0.121D-02 0.327D-02 0.611D-02

Coeff-Com: 0.825D-02-0.170D-01-0.576D-01-0.113D+00 0.272D+00 0.897D+00

Coeff: 0.488D-04-0.858D-04 0.375D-03 0.121D-02 0.327D-02 0.611D-02

Coeff: 0.825D-02-0.170D-01-0.576D-01-0.113D+00 0.272D+00 0.897D+00

Gap= 0.101 Goal= None Shift= 0.000

Gap= 0.051 Goal= None Shift= 0.000

RMSDP=1.85D-07 MaxDP=1.43D-05 DE=-3.89D-08 OVMax= 1.11D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 8.65D-08 CP: 9.80D-01 2.02D+00 7.31D-01 6.48D-01 7.34D-01

CP: 1.06D+00 1.50D+00 1.73D+00 1.16D+00 1.08D+00

CP: 1.34D+00 1.18D+00

E= -1914.19837365736 Delta-E= -0.000000021148 Rises=F Damp=F

DIIS: error= 3.75D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1914.19837365736 IErMin=13 ErrMin= 3.75D-06

ErrMax= 3.75D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.28D-09 BMatP= 2.44D-08

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

Coeff-Com: 0.379D-04-0.679D-04-0.694D-05 0.222D-03 0.110D-02 0.330D-02

Coeff-Com: 0.954D-02 0.295D-02-0.532D-01-0.144D+00 0.519D-02 0.456D+00

Coeff-Com: 0.719D+00

Coeff: 0.379D-04-0.679D-04-0.694D-05 0.222D-03 0.110D-02 0.330D-02

Coeff: 0.954D-02 0.295D-02-0.532D-01-0.144D+00 0.519D-02 0.456D+00

Coeff: 0.719D+00

Gap= 0.101 Goal= None Shift= 0.000

Gap= 0.051 Goal= None Shift= 0.000

RMSDP=9.58D-08 MaxDP=6.51D-06 DE=-2.11D-08 OVMax= 4.36D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 4.77D-08 CP: 9.80D-01 2.02D+00 7.31D-01 6.48D-01 7.34D-01

CP: 1.06D+00 1.50D+00 1.73D+00 1.17D+00 1.11D+00

CP: 1.46D+00 1.45D+00 1.15D+00

E= -1914.19837366316 Delta-E= -0.000000005800 Rises=F Damp=F

DIIS: error= 2.18D-06 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1914.19837366316 IErMin=14 ErrMin= 2.18D-06

ErrMax= 2.18D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.06D-09 BMatP= 7.28D-09

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

Coeff-Com: 0.216D-05-0.264D-05-0.146D-03-0.417D-03-0.818D-03-0.118D-02

Coeff-Com: 0.779D-03 0.797D-02 0.740D-03-0.171D-01-0.117D+00-0.164D+00

Coeff-Com: 0.375D+00 0.917D+00

Coeff: 0.216D-05-0.264D-05-0.146D-03-0.417D-03-0.818D-03-0.118D-02

Coeff: 0.779D-03 0.797D-02 0.740D-03-0.171D-01-0.117D+00-0.164D+00

Coeff: 0.375D+00 0.917D+00

Gap= 0.101 Goal= None Shift= 0.000

Gap= 0.051 Goal= None Shift= 0.000

RMSDP=6.93D-08 MaxDP=4.38D-06 DE=-5.80D-09 OVMax= 3.21D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 2.12D-08 CP: 9.80D-01 2.02D+00 7.31D-01 6.48D-01 7.34D-01

CP: 1.06D+00 1.50D+00 1.73D+00 1.18D+00 1.12D+00

CP: 1.55D+00 1.62D+00 1.57D+00 1.20D+00

E= -1914.19837366541 Delta-E= -0.000000002249 Rises=F Damp=F

DIIS: error= 5.71D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1914.19837366541 IErMin=15 ErrMin= 5.71D-07

ErrMax= 5.71D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.85D-10 BMatP= 2.06D-09

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

Coeff-Com: -0.660D-05 0.111D-04-0.132D-04-0.685D-04-0.229D-03-0.614D-03

Coeff-Com: -0.141D-02 0.426D-05 0.778D-02 0.212D-01-0.830D-02-0.716D-01

Coeff-Com: -0.846D-01 0.382D-01 0.110D+01

Coeff: -0.660D-05 0.111D-04-0.132D-04-0.685D-04-0.229D-03-0.614D-03

Coeff: -0.141D-02 0.426D-05 0.778D-02 0.212D-01-0.830D-02-0.716D-01

Coeff: -0.846D-01 0.382D-01 0.110D+01

Gap= 0.101 Goal= None Shift= 0.000

Gap= 0.051 Goal= None Shift= 0.000

RMSDP=2.49D-08 MaxDP=9.57D-07 DE=-2.25D-09 OVMax= 8.25D-06

Cycle 16 Pass 1 IDiag 1:

RMSU= 1.04D-08 CP: 9.80D-01 2.02D+00 7.31D-01 6.48D-01 7.34D-01

CP: 1.06D+00 1.50D+00 1.74D+00 1.18D+00 1.13D+00

CP: 1.57D+00 1.66D+00 1.71D+00 1.42D+00 1.49D+00

E= -1914.19837366570 Delta-E= -0.000000000286 Rises=F Damp=F

DIIS: error= 2.40D-07 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1914.19837366570 IErMin=16 ErrMin= 2.40D-07

ErrMax= 2.40D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.51D-11 BMatP= 1.85D-10

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

Coeff-Com: -0.429D-05 0.697D-05 0.277D-04 0.697D-04 0.912D-04 0.333D-04

Coeff-Com: -0.846D-03-0.178D-02 0.297D-02 0.132D-01 0.229D-01 0.762D-02

Coeff-Com: -0.131D+00-0.198D+00 0.558D+00 0.726D+00

Coeff: -0.429D-05 0.697D-05 0.277D-04 0.697D-04 0.912D-04 0.333D-04

Coeff: -0.846D-03-0.178D-02 0.297D-02 0.132D-01 0.229D-01 0.762D-02

Coeff: -0.131D+00-0.198D+00 0.558D+00 0.726D+00

Gap= 0.101 Goal= None Shift= 0.000

Gap= 0.051 Goal= None Shift= 0.000

RMSDP=1.10D-08 MaxDP=5.11D-07 DE=-2.86D-10 OVMax= 3.57D-06

Cycle 17 Pass 1 IDiag 1:

RMSU= 4.86D-09 CP: 9.80D-01 2.02D+00 7.31D-01 6.48D-01 7.34D-01

CP: 1.06D+00 1.50D+00 1.74D+00 1.18D+00 1.13D+00

CP: 1.57D+00 1.67D+00 1.75D+00 1.52D+00 1.81D+00

CP: 1.18D+00

E= -1914.19837366577 Delta-E= -0.000000000071 Rises=F Damp=F

DIIS: error= 1.15D-07 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=17 EnMin= -1914.19837366577 IErMin=17 ErrMin= 1.15D-07

ErrMax= 1.15D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.88D-11 BMatP= 9.51D-11

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

Coeff-Com: 0.674D-06-0.119D-05 0.153D-04 0.513D-04 0.102D-03 0.227D-03

Coeff-Com: -0.168D-04-0.662D-03-0.112D-02-0.697D-03 0.116D-01 0.237D-01

Coeff-Com: -0.273D-01-0.847D-01-0.119D+00 0.253D+00 0.945D+00

Coeff: 0.674D-06-0.119D-05 0.153D-04 0.513D-04 0.102D-03 0.227D-03

Coeff: -0.168D-04-0.662D-03-0.112D-02-0.697D-03 0.116D-01 0.237D-01

Coeff: -0.273D-01-0.847D-01-0.119D+00 0.253D+00 0.945D+00

Gap= 0.101 Goal= None Shift= 0.000

Gap= 0.051 Goal= None Shift= 0.000

RMSDP=6.82D-09 MaxDP=4.30D-07 DE=-7.09D-11 OVMax= 3.11D-06

Error on total polarization charges = 0.07963

SCF Done: E(UB3LYP) = -1914.19837367 A.U. after 17 cycles

NFock= 17 Conv=0.68D-08 -V/T= 2.0043

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7890 S= 0.5193

<L.S>= 0.000000000000E+00

KE= 1.906089589401D+03 PE=-1.513182195035D+04 EE= 5.952719155413D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.29

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7890, after 0.7512

Leave Link 502 at Sun Aug 18 13:47:42 2019, MaxMem= 2013265920 cpu: 3120.0

(Enter /home/kira/g09/l601.exe)

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

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Population analysis using the SCF density.

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Orbital symmetries:

Alpha Orbitals:

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The electronic state is 2-A1.

Alpha occ. eigenvalues -- -14.38183 -14.38183 -14.32207 -14.32207 -10.24622

Alpha occ. eigenvalues -- -10.24622 -10.24622 -10.24622 -10.23660 -10.23660

Alpha occ. eigenvalues -- -10.23660 -10.23660 -10.22635 -10.22635 -10.22635

Alpha occ. eigenvalues -- -10.22635 -10.20025 -10.20025 -10.20025 -10.20025

Alpha occ. eigenvalues -- -10.19499 -10.19499 -10.19435 -10.19435 -10.18404

Alpha occ. eigenvalues -- -10.18404 -10.18404 -10.18404 -10.18382 -10.18382

Alpha occ. eigenvalues -- -10.18382 -10.18382 -10.18076 -10.18076 -10.18076

Alpha occ. eigenvalues -- -10.18076 -10.17982 -10.17982 -10.17964 -10.17964

Alpha occ. eigenvalues -- -10.17964 -10.17964 -10.17950 -10.17950 -10.17950

Alpha occ. eigenvalues -- -10.17950 -10.17912 -10.17912 -1.01698 -1.01526

Alpha occ. eigenvalues -- -0.97344 -0.97027 -0.88773 -0.88018 -0.88000

Alpha occ. eigenvalues -- -0.87663 -0.84722 -0.83524 -0.83039 -0.82038

Alpha occ. eigenvalues -- -0.81390 -0.80387 -0.78214 -0.77807 -0.76026

Alpha occ. eigenvalues -- -0.75726 -0.75712 -0.75686 -0.75669 -0.75349

Alpha occ. eigenvalues -- -0.74882 -0.74364 -0.73017 -0.69020 -0.68573

Alpha occ. eigenvalues -- -0.63902 -0.62846 -0.62369 -0.62046 -0.61959

Alpha occ. eigenvalues -- -0.61708 -0.61651 -0.61612 -0.61403 -0.61151

Alpha occ. eigenvalues -- -0.60700 -0.60072 -0.58765 -0.57728 -0.56972

Alpha occ. eigenvalues -- -0.56411 -0.54679 -0.53730 -0.53290 -0.52533

Alpha occ. eigenvalues -- -0.52492 -0.51569 -0.51375 -0.50514 -0.48221

Alpha occ. eigenvalues -- -0.47929 -0.47543 -0.47219 -0.47043 -0.46926

Alpha occ. eigenvalues -- -0.46544 -0.46478 -0.46387 -0.45802 -0.45650

Alpha occ. eigenvalues -- -0.45090 -0.44800 -0.44372 -0.43976 -0.43852

Alpha occ. eigenvalues -- -0.43445 -0.43157 -0.43114 -0.42940 -0.42897

Alpha occ. eigenvalues -- -0.42875 -0.42489 -0.42015 -0.41578 -0.41280

Alpha occ. eigenvalues -- -0.41014 -0.40322 -0.39852 -0.39663 -0.39138

Alpha occ. eigenvalues -- -0.37808 -0.37798 -0.37528 -0.37281 -0.36213

Alpha occ. eigenvalues -- -0.36075 -0.35928 -0.35785 -0.35504 -0.35503

Alpha occ. eigenvalues -- -0.35438 -0.35431 -0.34343 -0.31546 -0.30915

Alpha occ. eigenvalues -- -0.30287 -0.30218 -0.29059 -0.29007 -0.27605

Alpha occ. eigenvalues -- -0.26938 -0.26900 -0.26708 -0.26571 -0.26355

Alpha occ. eigenvalues -- -0.26345 -0.26285 -0.26210 -0.26203 -0.22524

Alpha occ. eigenvalues -- -0.22135

Alpha virt. eigenvalues -- -0.11998 -0.11694 -0.05727 -0.02395 -0.02330

Alpha virt. eigenvalues -- -0.02272 -0.02091 -0.01875 -0.01792 -0.01741

Alpha virt. eigenvalues -- -0.01722 0.00925 0.03536 0.03837 0.05001

Alpha virt. eigenvalues -- 0.05312 0.05333 0.05393 0.05827 0.06796

Alpha virt. eigenvalues -- 0.07963 0.08071 0.08208 0.08483 0.08999

Alpha virt. eigenvalues -- 0.09068 0.09091 0.09522 0.09553 0.09735

Alpha virt. eigenvalues -- 0.10004 0.10013 0.10048 0.10084 0.10201

Alpha virt. eigenvalues -- 0.10601 0.12097 0.12266 0.12342 0.12609

Alpha virt. eigenvalues -- 0.12742 0.12994 0.13009 0.13443 0.13536

Alpha virt. eigenvalues -- 0.13619 0.13667 0.13730 0.13806 0.14095

Alpha virt. eigenvalues -- 0.14346 0.14488 0.15204 0.15839 0.16599

Alpha virt. eigenvalues -- 0.19559 0.20187 0.20976 0.21014 0.21720

Alpha virt. eigenvalues -- 0.22069 0.22709 0.23001 0.23490 0.24175

Alpha virt. eigenvalues -- 0.24276 0.24613 0.24969 0.25108 0.26040

Alpha virt. eigenvalues -- 0.26572 0.27078 0.27421 0.27462 0.27476

Alpha virt. eigenvalues -- 0.27569 0.28037 0.28123 0.28680 0.28887

Alpha virt. eigenvalues -- 0.28887 0.28994 0.29290 0.29381 0.29615

Alpha virt. eigenvalues -- 0.29866 0.29890 0.30314 0.30444 0.31937

Alpha virt. eigenvalues -- 0.32506 0.33330 0.33821 0.34216 0.34314

Alpha virt. eigenvalues -- 0.34330 0.34751 0.34873 0.35018 0.35306

Alpha virt. eigenvalues -- 0.35343 0.35488 0.35959 0.35979 0.36202

Alpha virt. eigenvalues -- 0.36722 0.37285 0.37486 0.38155 0.38350

Alpha virt. eigenvalues -- 0.38519 0.38613 0.38619 0.39331 0.39420

Alpha virt. eigenvalues -- 0.39775 0.39997 0.40218 0.40254 0.40432

Alpha virt. eigenvalues -- 0.40439 0.40827 0.40883 0.40940 0.41185

Alpha virt. eigenvalues -- 0.41210 0.41461 0.41487 0.42060 0.42136

Alpha virt. eigenvalues -- 0.42323 0.42384 0.42733 0.42899 0.42992

Alpha virt. eigenvalues -- 0.43658 0.43682 0.43800 0.43811 0.44039

Alpha virt. eigenvalues -- 0.44291 0.44437 0.44509 0.44608 0.44614

Alpha virt. eigenvalues -- 0.44843 0.45582 0.45634 0.46288 0.46320

Alpha virt. eigenvalues -- 0.46622 0.46739 0.47128 0.47642 0.47812

Alpha virt. eigenvalues -- 0.48376 0.48708 0.48726 0.49243 0.49711

Alpha virt. eigenvalues -- 0.49783 0.49910 0.50349 0.50893 0.51958

Alpha virt. eigenvalues -- 0.52160 0.52257 0.53110 0.53382 0.53391

Alpha virt. eigenvalues -- 0.53403 0.53626 0.55270 0.55293 0.56290

Alpha virt. eigenvalues -- 0.56488 0.56642 0.56710 0.56798 0.56890

Alpha virt. eigenvalues -- 0.57324 0.58084 0.58714 0.59045 0.59594

Alpha virt. eigenvalues -- 0.59596 0.59675 0.59748 0.59869 0.60318

Alpha virt. eigenvalues -- 0.60379 0.60402 0.60528 0.60543 0.60807

Alpha virt. eigenvalues -- 0.60837 0.60880 0.61157 0.61228 0.61488

Alpha virt. eigenvalues -- 0.61581 0.62813 0.62871 0.63185 0.63470

Alpha virt. eigenvalues -- 0.63923 0.63934 0.64065 0.64126 0.64566

Alpha virt. eigenvalues -- 0.64567 0.64906 0.65189 0.65580 0.66019

Alpha virt. eigenvalues -- 0.66068 0.66126 0.67101 0.67542 0.68028

Alpha virt. eigenvalues -- 0.68045 0.68450 0.68945 0.69139 0.69598

Alpha virt. eigenvalues -- 0.69623 0.71211 0.71370 0.71616 0.71727

Alpha virt. eigenvalues -- 0.71950 0.72112 0.72353 0.72762 0.73184

Alpha virt. eigenvalues -- 0.73288 0.73910 0.74470 0.74546 0.74679

Alpha virt. eigenvalues -- 0.74849 0.75109 0.75483 0.75902 0.76088

Alpha virt. eigenvalues -- 0.76311 0.76708 0.76784 0.77833 0.78553

Alpha virt. eigenvalues -- 0.78598 0.78714 0.79131 0.79219 0.79795

Alpha virt. eigenvalues -- 0.80046 0.80087 0.80087 0.80522 0.80938

Alpha virt. eigenvalues -- 0.81148 0.81250 0.82136 0.83060 0.84012

Alpha virt. eigenvalues -- 0.84598 0.84605 0.85222 0.86054 0.86070

Alpha virt. eigenvalues -- 0.86200 0.86282 0.87896 0.88005 0.88125

Alpha virt. eigenvalues -- 0.88267 0.88509 0.88705 0.89760 0.90669

Alpha virt. eigenvalues -- 0.90984 0.91183 0.91336 0.91859 0.91887

Alpha virt. eigenvalues -- 0.93817 0.93898 0.94368 0.95346 0.95818

Alpha virt. eigenvalues -- 0.95909 0.96449 0.97242 0.97875 0.97891

Alpha virt. eigenvalues -- 0.98612 0.98944 1.00613 1.00668 1.00691

Alpha virt. eigenvalues -- 1.00965 1.01613 1.02114 1.03277 1.03467

Alpha virt. eigenvalues -- 1.03940 1.04769 1.05028 1.06459 1.06840

Alpha virt. eigenvalues -- 1.07346 1.07688 1.07932 1.08748 1.08943

Alpha virt. eigenvalues -- 1.09249 1.10087 1.11625 1.12181 1.12268

Alpha virt. eigenvalues -- 1.12367 1.13318 1.13887 1.13991 1.14408

Alpha virt. eigenvalues -- 1.14676 1.15304 1.15832 1.16118 1.16552

Alpha virt. eigenvalues -- 1.17052 1.17986 1.18704 1.18827 1.19026

Alpha virt. eigenvalues -- 1.19412 1.19788 1.19884 1.20003 1.20003

Alpha virt. eigenvalues -- 1.20764 1.21442 1.22130 1.22275 1.22958

Alpha virt. eigenvalues -- 1.23234 1.23328 1.23599 1.23822 1.23990

Alpha virt. eigenvalues -- 1.24459 1.24519 1.24604 1.25788 1.25819

Alpha virt. eigenvalues -- 1.26102 1.26848 1.27318 1.27817 1.28995

Alpha virt. eigenvalues -- 1.29787 1.29968 1.30784 1.31921 1.32219

Alpha virt. eigenvalues -- 1.36194 1.36568 1.37208 1.38012 1.38470

Alpha virt. eigenvalues -- 1.38957 1.39078 1.41426 1.41468 1.41815

Alpha virt. eigenvalues -- 1.41818 1.43030 1.43372 1.43673 1.46031

Alpha virt. eigenvalues -- 1.46194 1.46383 1.46444 1.46723 1.46742

Alpha virt. eigenvalues -- 1.47616 1.47832 1.48058 1.48155 1.48181

Alpha virt. eigenvalues -- 1.48409 1.50281 1.52116 1.52663 1.52754

Alpha virt. eigenvalues -- 1.52963 1.53176 1.53273 1.53329 1.55800

Alpha virt. eigenvalues -- 1.55832 1.56012 1.57197 1.59568 1.59927

Alpha virt. eigenvalues -- 1.60396 1.60805 1.61014 1.62163 1.64227

Alpha virt. eigenvalues -- 1.64294 1.65487 1.65525 1.66223 1.66827

Alpha virt. eigenvalues -- 1.67682 1.68414 1.68692 1.69130 1.69543

Alpha virt. eigenvalues -- 1.70183 1.70557 1.72467 1.72573 1.73450

Alpha virt. eigenvalues -- 1.73790 1.74029 1.74721 1.74773 1.74839

Alpha virt. eigenvalues -- 1.74888 1.75408 1.76154 1.76243 1.77863

Alpha virt. eigenvalues -- 1.78113 1.78520 1.78979 1.79370 1.79484

Alpha virt. eigenvalues -- 1.80118 1.80347 1.80910 1.81192 1.81926

Alpha virt. eigenvalues -- 1.82134 1.82752 1.83264 1.83512 1.83659

Alpha virt. eigenvalues -- 1.83997 1.84573 1.85795 1.86056 1.86299

Alpha virt. eigenvalues -- 1.86658 1.86716 1.87221 1.87939 1.88639

Alpha virt. eigenvalues -- 1.89790 1.89862 1.89918 1.90217 1.90856

Alpha virt. eigenvalues -- 1.91353 1.91389 1.91429 1.91750 1.91903

Alpha virt. eigenvalues -- 1.92291 1.92827 1.92886 1.93049 1.93149

Alpha virt. eigenvalues -- 1.93264 1.93397 1.94360 1.94498 1.94697

Alpha virt. eigenvalues -- 1.95241 1.95370 1.95634 1.96502 1.96761

Alpha virt. eigenvalues -- 1.97962 1.98340 1.98821 1.99208 1.99236

Alpha virt. eigenvalues -- 2.01623 2.05484 2.05717 2.05928 2.06014

Alpha virt. eigenvalues -- 2.06571 2.06629 2.07342 2.09170 2.11668

Alpha virt. eigenvalues -- 2.11915 2.12128 2.15644 2.17747 2.20548

Alpha virt. eigenvalues -- 2.22409 2.22995 2.23104 2.24088 2.24163

Alpha virt. eigenvalues -- 2.24776 2.25506 2.25696 2.25860 2.25943

Alpha virt. eigenvalues -- 2.26162 2.26646 2.26947 2.26971 2.27084

Alpha virt. eigenvalues -- 2.27327 2.27423 2.28077 2.28890 2.28915

Alpha virt. eigenvalues -- 2.28977 2.30173 2.30278 2.30810 2.31196

Alpha virt. eigenvalues -- 2.31429 2.31896 2.32574 2.33029 2.33713

Alpha virt. eigenvalues -- 2.34142 2.34507 2.34893 2.34918 2.35523

Alpha virt. eigenvalues -- 2.35567 2.36643 2.37021 2.37404 2.37417

Alpha virt. eigenvalues -- 2.39102 2.39721 2.40061 2.41089 2.42350

Alpha virt. eigenvalues -- 2.43001 2.45691 2.45985 2.47518 2.48172

Alpha virt. eigenvalues -- 2.50429 2.50691 2.51277 2.51741 2.52359

Alpha virt. eigenvalues -- 2.52548 2.54209 2.55553 2.55895 2.56240

Alpha virt. eigenvalues -- 2.57190 2.57604 2.58835 2.58910 2.59373

Alpha virt. eigenvalues -- 2.59594 2.59728 2.59874 2.60591 2.60855

Alpha virt. eigenvalues -- 2.63155 2.63602 2.64149 2.64715 2.65549

Alpha virt. eigenvalues -- 2.65973 2.67228 2.68484 2.68701 2.69433

Alpha virt. eigenvalues -- 2.69563 2.70503 2.71604 2.72010 2.72658

Alpha virt. eigenvalues -- 2.72810 2.73802 2.74098 2.74976 2.74977

Alpha virt. eigenvalues -- 2.75750 2.77768 2.78425 2.78466 2.78573

Alpha virt. eigenvalues -- 2.78880 2.79046 2.80612 2.81177 2.82268

Alpha virt. eigenvalues -- 2.83292 2.84252 2.84325 2.84581 2.85968

Alpha virt. eigenvalues -- 2.87193 2.88097 2.88649 2.89094 2.91267

Alpha virt. eigenvalues -- 2.93627 2.94665 2.94772 2.95243 2.96590

Alpha virt. eigenvalues -- 2.96870 2.96909 2.97477 3.00492 3.01169

Alpha virt. eigenvalues -- 3.01226 3.02164 3.02998 3.03660 3.05189

Alpha virt. eigenvalues -- 3.05860 3.06089 3.06420 3.06586 3.06642

Alpha virt. eigenvalues -- 3.08927 3.09133 3.10679 3.10808 3.12186

Alpha virt. eigenvalues -- 3.13182 3.13571 3.14453 3.14729 3.16984

Alpha virt. eigenvalues -- 3.17747 3.18247 3.20284 3.20777 3.21220

Alpha virt. eigenvalues -- 3.24102 3.25299 3.25489 3.25522 3.25933

Alpha virt. eigenvalues -- 3.26650 3.28212 3.28330 3.28424 3.28678

Alpha virt. eigenvalues -- 3.29012 3.29409 3.29494 3.29772 3.30110

Alpha virt. eigenvalues -- 3.30140 3.30351 3.30492 3.30524 3.31302

Alpha virt. eigenvalues -- 3.32572 3.33020 3.33196 3.33518 3.35292

Alpha virt. eigenvalues -- 3.35466 3.37533 3.37693 3.39279 3.39675

Alpha virt. eigenvalues -- 3.40055 3.41237 3.41630 3.43032 3.43671

Alpha virt. eigenvalues -- 3.49407 3.50697 3.50755 3.51385 3.55479

Alpha virt. eigenvalues -- 3.55831 3.56690 3.57127 3.57308 3.58830

Alpha virt. eigenvalues -- 3.58895 3.60432 3.61654 3.64318 3.64486

Alpha virt. eigenvalues -- 3.66380 3.70953 3.71047 3.72139 3.74193

Alpha virt. eigenvalues -- 3.74749 3.77230 3.78684 3.79514 3.79944

Alpha virt. eigenvalues -- 3.81988 3.83572 3.85955 3.90799 3.93685

Alpha virt. eigenvalues -- 3.93925 3.94327 3.94885 3.95082 3.95166

Alpha virt. eigenvalues -- 3.95418 3.97366 3.97741 4.01822 4.09639

Alpha virt. eigenvalues -- 4.27005 4.28649 4.34483 4.38156 4.43934

Alpha virt. eigenvalues -- 4.48911 4.52933 4.54580 4.62292 4.62360

Alpha virt. eigenvalues -- 4.65704 4.67529 4.77931 4.77941 4.77946

Alpha virt. eigenvalues -- 4.77956 5.07258 5.13710 5.16164 5.29074

Alpha virt. eigenvalues -- 23.24260 23.27919 23.28241 23.29848 23.43743

Alpha virt. eigenvalues -- 23.50403 23.50723 23.56307 23.71048 23.72198

Alpha virt. eigenvalues -- 23.74719 23.75733 23.80215 23.80370 23.80370

Alpha virt. eigenvalues -- 23.80623 23.84082 23.84991 23.85057 23.85784

Alpha virt. eigenvalues -- 23.91401 23.91853 23.93587 23.95581 23.96945

Alpha virt. eigenvalues -- 23.97526 23.98294 23.98716 24.03929 24.04043

Alpha virt. eigenvalues -- 24.04129 24.04246 24.07667 24.07841 24.08716

Alpha virt. eigenvalues -- 24.08890 24.10893 24.10991 24.14910 24.15144

Alpha virt. eigenvalues -- 24.15480 24.15495 24.15535 24.15560 35.53512

Alpha virt. eigenvalues -- 35.54465 35.60587 35.61212

Beta occ. eigenvalues -- -14.38034 -14.38033 -14.31883 -14.31883 -10.24684

Beta occ. eigenvalues -- -10.24684 -10.24684 -10.24683 -10.23326 -10.23326

Beta occ. eigenvalues -- -10.23326 -10.23326 -10.22744 -10.22744 -10.22744

Beta occ. eigenvalues -- -10.22744 -10.20046 -10.20045 -10.20045 -10.20045

Beta occ. eigenvalues -- -10.19486 -10.19486 -10.19422 -10.19422 -10.18371

Beta occ. eigenvalues -- -10.18371 -10.18371 -10.18371 -10.18349 -10.18349

Beta occ. eigenvalues -- -10.18349 -10.18349 -10.18058 -10.18058 -10.18058

Beta occ. eigenvalues -- -10.18058 -10.17997 -10.17997 -10.17971 -10.17971

Beta occ. eigenvalues -- -10.17971 -10.17971 -10.17954 -10.17954 -10.17954

Beta occ. eigenvalues -- -10.17954 -10.17927 -10.17927 -1.01516 -1.01354

Beta occ. eigenvalues -- -0.97008 -0.96706 -0.88513 -0.87849 -0.87817

Beta occ. eigenvalues -- -0.87530 -0.84496 -0.83206 -0.82705 -0.81814

Beta occ. eigenvalues -- -0.81291 -0.80071 -0.78085 -0.77675 -0.76007

Beta occ. eigenvalues -- -0.75688 -0.75672 -0.75646 -0.75625 -0.75295

Beta occ. eigenvalues -- -0.74830 -0.74425 -0.72705 -0.68799 -0.68410

Beta occ. eigenvalues -- -0.63777 -0.62759 -0.62319 -0.61980 -0.61900

Beta occ. eigenvalues -- -0.61673 -0.61590 -0.61545 -0.61331 -0.61080

Beta occ. eigenvalues -- -0.60632 -0.59965 -0.58736 -0.57662 -0.56948

Beta occ. eigenvalues -- -0.56335 -0.54554 -0.53645 -0.53246 -0.52487

Beta occ. eigenvalues -- -0.52428 -0.51463 -0.51301 -0.50378 -0.48074

Beta occ. eigenvalues -- -0.47857 -0.47197 -0.46987 -0.46933 -0.46767

Beta occ. eigenvalues -- -0.46427 -0.46356 -0.46317 -0.45725 -0.45595

Beta occ. eigenvalues -- -0.44845 -0.44557 -0.44329 -0.43928 -0.43812

Beta occ. eigenvalues -- -0.43370 -0.43082 -0.43035 -0.42919 -0.42871

Beta occ. eigenvalues -- -0.42851 -0.42221 -0.41844 -0.41207 -0.41194

Beta occ. eigenvalues -- -0.40971 -0.40255 -0.39833 -0.39647 -0.39125

Beta occ. eigenvalues -- -0.37730 -0.37728 -0.37461 -0.37124 -0.36144

Beta occ. eigenvalues -- -0.35854 -0.35707 -0.35698 -0.35417 -0.35415

Beta occ. eigenvalues -- -0.35381 -0.35347 -0.33655 -0.30675 -0.29965

Beta occ. eigenvalues -- -0.29947 -0.29904 -0.28593 -0.28507 -0.27268

Beta occ. eigenvalues -- -0.26667 -0.26652 -0.26638 -0.26510 -0.26217

Beta occ. eigenvalues -- -0.26193 -0.26013 -0.25818 -0.25634 -0.22756

Beta virt. eigenvalues -- -0.17672 -0.10715 -0.10397 -0.04849 -0.02310

Beta virt. eigenvalues -- -0.02266 -0.02190 -0.01994 -0.01826 -0.01722

Beta virt. eigenvalues -- -0.01677 -0.01640 0.01407 0.03583 0.03980

Beta virt. eigenvalues -- 0.05027 0.05330 0.05343 0.05350 0.05759

Beta virt. eigenvalues -- 0.06863 0.07973 0.08084 0.08213 0.08675

Beta virt. eigenvalues -- 0.09070 0.09072 0.09097 0.09541 0.09767

Beta virt. eigenvalues -- 0.09878 0.10018 0.10083 0.10083 0.10242

Beta virt. eigenvalues -- 0.10680 0.11048 0.12104 0.12262 0.12347

Beta virt. eigenvalues -- 0.12684 0.12742 0.13056 0.13062 0.13485

Beta virt. eigenvalues -- 0.13635 0.13636 0.13681 0.13776 0.13823

Beta virt. eigenvalues -- 0.14227 0.14447 0.14688 0.15340 0.15923

Beta virt. eigenvalues -- 0.16687 0.19644 0.20215 0.21077 0.21103

Beta virt. eigenvalues -- 0.21844 0.22186 0.22977 0.23081 0.23659

Beta virt. eigenvalues -- 0.24244 0.24325 0.24647 0.24986 0.25092

Beta virt. eigenvalues -- 0.26041 0.26702 0.27163 0.27436 0.27477

Beta virt. eigenvalues -- 0.27491 0.27581 0.28116 0.28154 0.28717

Beta virt. eigenvalues -- 0.28916 0.28959 0.29033 0.29334 0.29407

Beta virt. eigenvalues -- 0.29667 0.29894 0.29923 0.30388 0.30472

Beta virt. eigenvalues -- 0.31965 0.32577 0.33444 0.34055 0.34270

Beta virt. eigenvalues -- 0.34355 0.34370 0.34964 0.35048 0.35209

Beta virt. eigenvalues -- 0.35458 0.35571 0.35626 0.36010 0.36016

Beta virt. eigenvalues -- 0.36506 0.36839 0.37428 0.37539 0.38276

Beta virt. eigenvalues -- 0.38394 0.38559 0.38655 0.38742 0.39313

Beta virt. eigenvalues -- 0.39440 0.39833 0.40085 0.40310 0.40311

Beta virt. eigenvalues -- 0.40462 0.40471 0.40899 0.40900 0.41047

Beta virt. eigenvalues -- 0.41238 0.41245 0.41541 0.41544 0.42085

Beta virt. eigenvalues -- 0.42181 0.42356 0.42416 0.42801 0.42923

Beta virt. eigenvalues -- 0.43007 0.43710 0.43713 0.43847 0.43890

Beta virt. eigenvalues -- 0.44081 0.44296 0.44490 0.44592 0.44644

Beta virt. eigenvalues -- 0.44654 0.44869 0.45643 0.45686 0.46293

Beta virt. eigenvalues -- 0.46473 0.46668 0.46832 0.47291 0.47693

Beta virt. eigenvalues -- 0.47835 0.48414 0.48726 0.48932 0.49226

Beta virt. eigenvalues -- 0.49782 0.49842 0.49943 0.50273 0.50960

Beta virt. eigenvalues -- 0.52021 0.52307 0.52335 0.53172 0.53429

Beta virt. eigenvalues -- 0.53430 0.53441 0.53694 0.55305 0.55332

Beta virt. eigenvalues -- 0.56380 0.56594 0.56669 0.56773 0.56826

Beta virt. eigenvalues -- 0.56965 0.57378 0.58270 0.58756 0.59077

Beta virt. eigenvalues -- 0.59615 0.59649 0.59700 0.59781 0.59984

Beta virt. eigenvalues -- 0.60357 0.60422 0.60442 0.60496 0.60548

Beta virt. eigenvalues -- 0.60830 0.60873 0.60959 0.61307 0.61343

Beta virt. eigenvalues -- 0.61563 0.61669 0.62968 0.63030 0.63272

Beta virt. eigenvalues -- 0.63510 0.63889 0.63951 0.64150 0.64159

Beta virt. eigenvalues -- 0.64591 0.64652 0.64978 0.65254 0.65684

Beta virt. eigenvalues -- 0.66065 0.66093 0.66119 0.67092 0.67894

Beta virt. eigenvalues -- 0.68085 0.68147 0.68591 0.69094 0.69310

Beta virt. eigenvalues -- 0.69656 0.69718 0.71326 0.71461 0.71672

Beta virt. eigenvalues -- 0.71810 0.71957 0.72233 0.72394 0.72943

Beta virt. eigenvalues -- 0.73256 0.73429 0.73973 0.74534 0.74609

Beta virt. eigenvalues -- 0.74707 0.74866 0.75102 0.75554 0.75931

Beta virt. eigenvalues -- 0.76340 0.76445 0.76820 0.77096 0.77884

Beta virt. eigenvalues -- 0.78588 0.78716 0.78746 0.79156 0.79247

Beta virt. eigenvalues -- 0.79856 0.80071 0.80148 0.80299 0.80551

Beta virt. eigenvalues -- 0.81007 0.81265 0.81339 0.82171 0.83273

Beta virt. eigenvalues -- 0.84078 0.84628 0.84744 0.85244 0.86109

Beta virt. eigenvalues -- 0.86175 0.86246 0.86308 0.87985 0.88110

Beta virt. eigenvalues -- 0.88224 0.88374 0.88565 0.88829 0.89846

Beta virt. eigenvalues -- 0.90732 0.91148 0.91332 0.91448 0.91934

Beta virt. eigenvalues -- 0.92023 0.93922 0.94009 0.94448 0.95352

Beta virt. eigenvalues -- 0.95880 0.95963 0.96506 0.97329 0.97902

Beta virt. eigenvalues -- 0.97983 0.98676 0.99070 1.00694 1.00726

Beta virt. eigenvalues -- 1.00728 1.01139 1.01716 1.02150 1.03517

Beta virt. eigenvalues -- 1.03579 1.04073 1.04850 1.05080 1.06575

Beta virt. eigenvalues -- 1.06966 1.07433 1.07850 1.07976 1.08872

Beta virt. eigenvalues -- 1.09067 1.09432 1.10170 1.11811 1.12293

Beta virt. eigenvalues -- 1.12321 1.12406 1.13398 1.13946 1.14032

Beta virt. eigenvalues -- 1.14469 1.14733 1.15319 1.15861 1.16148

Beta virt. eigenvalues -- 1.16572 1.17048 1.18053 1.18767 1.18849

Beta virt. eigenvalues -- 1.19060 1.19389 1.19861 1.19945 1.20053

Beta virt. eigenvalues -- 1.20057 1.20840 1.21492 1.22175 1.22349

Beta virt. eigenvalues -- 1.23047 1.23248 1.23468 1.23650 1.23870

Beta virt. eigenvalues -- 1.24086 1.24538 1.24612 1.24701 1.25842

Beta virt. eigenvalues -- 1.25847 1.26195 1.27055 1.27441 1.28012

Beta virt. eigenvalues -- 1.29080 1.29995 1.30123 1.30823 1.31968

Beta virt. eigenvalues -- 1.32245 1.36298 1.36716 1.37338 1.38322

Beta virt. eigenvalues -- 1.38718 1.39178 1.39285 1.41490 1.41510

Beta virt. eigenvalues -- 1.41839 1.41973 1.43225 1.43618 1.43734

Beta virt. eigenvalues -- 1.46117 1.46255 1.46513 1.46527 1.46796

Beta virt. eigenvalues -- 1.46841 1.47655 1.47885 1.48111 1.48203

Beta virt. eigenvalues -- 1.48261 1.48474 1.50346 1.52165 1.52724

Beta virt. eigenvalues -- 1.52804 1.53228 1.53322 1.53327 1.53389

Beta virt. eigenvalues -- 1.55884 1.56131 1.56309 1.57235 1.59778

Beta virt. eigenvalues -- 1.59944 1.60504 1.60859 1.61089 1.62173

Beta virt. eigenvalues -- 1.64294 1.64364 1.65655 1.65779 1.66296

Beta virt. eigenvalues -- 1.66940 1.67738 1.68501 1.68808 1.69256

Beta virt. eigenvalues -- 1.69673 1.70251 1.70602 1.72515 1.72850

Beta virt. eigenvalues -- 1.73535 1.74033 1.74166 1.74819 1.74912

Beta virt. eigenvalues -- 1.74975 1.75056 1.75594 1.76196 1.76337

Beta virt. eigenvalues -- 1.77984 1.78335 1.78569 1.79030 1.79221

Beta virt. eigenvalues -- 1.79532 1.80199 1.80326 1.80942 1.81280

Beta virt. eigenvalues -- 1.81947 1.82172 1.82787 1.83352 1.83587

Beta virt. eigenvalues -- 1.83718 1.84063 1.84630 1.85909 1.86193

Beta virt. eigenvalues -- 1.86503 1.86794 1.86908 1.87283 1.87989

Beta virt. eigenvalues -- 1.88668 1.89850 1.89977 1.90196 1.90250

Beta virt. eigenvalues -- 1.90863 1.91431 1.91454 1.91547 1.91778

Beta virt. eigenvalues -- 1.91932 1.92337 1.92887 1.92916 1.93094

Beta virt. eigenvalues -- 1.93169 1.93283 1.93449 1.94540 1.94543

Beta virt. eigenvalues -- 1.94766 1.95392 1.95437 1.95700 1.96609

Beta virt. eigenvalues -- 1.96836 1.98101 1.98425 1.98887 1.99210

Beta virt. eigenvalues -- 1.99274 2.01718 2.05644 2.05956 2.06062

Beta virt. eigenvalues -- 2.06074 2.06798 2.06881 2.07466 2.09244

Beta virt. eigenvalues -- 2.11711 2.12035 2.12218 2.16093 2.17683

Beta virt. eigenvalues -- 2.20578 2.22458 2.23067 2.23140 2.24282

Beta virt. eigenvalues -- 2.24292 2.24867 2.25594 2.25734 2.25950

Beta virt. eigenvalues -- 2.26067 2.26194 2.26682 2.27007 2.27096

Beta virt. eigenvalues -- 2.27147 2.27350 2.27523 2.28118 2.28931

Beta virt. eigenvalues -- 2.28983 2.29046 2.30233 2.30433 2.30896

Beta virt. eigenvalues -- 2.31214 2.31486 2.31926 2.32657 2.33131

Beta virt. eigenvalues -- 2.33930 2.34331 2.34527 2.34965 2.35033

Beta virt. eigenvalues -- 2.35647 2.35728 2.36670 2.37312 2.37439

Beta virt. eigenvalues -- 2.37522 2.39256 2.39768 2.40116 2.41306

Beta virt. eigenvalues -- 2.42499 2.43222 2.45815 2.46169 2.47667

Beta virt. eigenvalues -- 2.48349 2.50913 2.50969 2.51530 2.52072

Beta virt. eigenvalues -- 2.52580 2.52852 2.54305 2.55819 2.56018

Beta virt. eigenvalues -- 2.56551 2.57209 2.57948 2.58875 2.59296

Beta virt. eigenvalues -- 2.59517 2.59651 2.59862 2.59868 2.60867

Beta virt. eigenvalues -- 2.61035 2.63277 2.63737 2.64187 2.64736

Beta virt. eigenvalues -- 2.65752 2.66177 2.67526 2.68579 2.68728

Beta virt. eigenvalues -- 2.69495 2.69594 2.70633 2.71751 2.72085

Beta virt. eigenvalues -- 2.72942 2.72947 2.73918 2.74122 2.75056

Beta virt. eigenvalues -- 2.75143 2.75804 2.77856 2.78514 2.78547

Beta virt. eigenvalues -- 2.78673 2.78843 2.79102 2.80584 2.81069

Beta virt. eigenvalues -- 2.82374 2.83230 2.84342 2.84347 2.84672

Beta virt. eigenvalues -- 2.86008 2.87254 2.88111 2.88659 2.89096

Beta virt. eigenvalues -- 2.91292 2.93680 2.94718 2.94814 2.95277

Beta virt. eigenvalues -- 2.96791 2.96940 2.97598 2.97894 3.00558

Beta virt. eigenvalues -- 3.01121 3.01225 3.02892 3.03606 3.03728

Beta virt. eigenvalues -- 3.05219 3.06113 3.06199 3.06554 3.06736

Beta virt. eigenvalues -- 3.06819 3.09156 3.09403 3.10718 3.10849

Beta virt. eigenvalues -- 3.12212 3.13182 3.13659 3.14492 3.14766

Beta virt. eigenvalues -- 3.17012 3.17792 3.18304 3.20337 3.20790

Beta virt. eigenvalues -- 3.21225 3.24164 3.25310 3.25502 3.25534

Beta virt. eigenvalues -- 3.25972 3.26673 3.28244 3.28365 3.28454

Beta virt. eigenvalues -- 3.28799 3.29023 3.29442 3.29503 3.29783

Beta virt. eigenvalues -- 3.30156 3.30240 3.30386 3.30508 3.30540

Beta virt. eigenvalues -- 3.31323 3.32710 3.33074 3.33250 3.33698

Beta virt. eigenvalues -- 3.35438 3.35495 3.37561 3.37701 3.39296

Beta virt. eigenvalues -- 3.39708 3.40117 3.41260 3.41660 3.43081

Beta virt. eigenvalues -- 3.43691 3.49455 3.50725 3.50795 3.51418

Beta virt. eigenvalues -- 3.55498 3.55857 3.56700 3.57150 3.57330

Beta virt. eigenvalues -- 3.58846 3.58877 3.60422 3.61729 3.64344

Beta virt. eigenvalues -- 3.64535 3.66417 3.70981 3.71086 3.72203

Beta virt. eigenvalues -- 3.74281 3.75378 3.77261 3.79184 3.79568

Beta virt. eigenvalues -- 3.79972 3.81998 3.84936 3.87148 3.90941

Beta virt. eigenvalues -- 3.93792 3.94023 3.94383 3.94919 3.95153

Beta virt. eigenvalues -- 3.95190 3.95444 3.97489 3.97787 4.01938

Beta virt. eigenvalues -- 4.09727 4.27234 4.28886 4.34742 4.38433

Beta virt. eigenvalues -- 4.44141 4.49129 4.53022 4.54783 4.62512

Beta virt. eigenvalues -- 4.62611 4.65775 4.67665 4.77963 4.77973

Beta virt. eigenvalues -- 4.77978 4.77988 5.07359 5.13798 5.16361

Beta virt. eigenvalues -- 5.29260 23.24279 23.27934 23.28256 23.29862

Beta virt. eigenvalues -- 23.43772 23.50403 23.50756 23.56300 23.71122

Beta virt. eigenvalues -- 23.72269 23.74784 23.75809 23.80231 23.80386

Beta virt. eigenvalues -- 23.80386 23.80638 23.84099 23.85007 23.85075

Beta virt. eigenvalues -- 23.85802 23.91316 23.91781 23.93551 23.95510

Beta virt. eigenvalues -- 23.97060 23.97612 23.98353 23.98760 24.03944

Beta virt. eigenvalues -- 24.04058 24.04143 24.04261 24.07739 24.07912

Beta virt. eigenvalues -- 24.08798 24.08971 24.10912 24.11009 24.14891

Beta virt. eigenvalues -- 24.15125 24.15518 24.15533 24.15574 24.15600

Beta virt. eigenvalues -- 35.53668 35.54621 35.60930 35.61556

Condensed to atoms (all electrons):

Atomic-Atomic Spin Densities.

Mulliken charges and spin densities:

1 2

1 C -0.232866 0.011269

2 C 0.375669 -0.045380

3 N -0.696351 0.071162

4 C 0.375669 -0.045380

5 C -0.232866 0.011269

6 C -0.058506 0.240844

7 C 0.241049 -0.078041

8 N -0.484908 0.160011

9 C 0.241049 -0.078041

10 C -0.230673 -0.009834

11 C -0.230673 -0.009834

12 C -0.058506 0.240844

13 C 0.241049 -0.078041

14 C -0.230673 -0.009834

15 C -0.230673 -0.009834

16 C 0.241049 -0.078041

17 N -0.484908 0.160011

18 C -0.058506 0.240844

19 C 0.375669 -0.045380

20 C -0.232866 0.011269

21 C -0.232866 0.011269

22 C 0.375669 -0.045380

23 N -0.696351 0.071162

24 C -0.058506 0.240844

25 C -0.138257 -0.019788

26 C -0.195786 0.017384

27 C -0.212352 -0.006939

28 C -0.209418 0.016595

29 C -0.212426 -0.006634

30 C -0.193168 0.017299

31 C -0.209418 0.016595

32 C -0.212352 -0.006939

33 C -0.195786 0.017384

34 C -0.138257 -0.019788

35 C -0.193168 0.017299

36 C -0.212426 -0.006634

37 C -0.138257 -0.019788

38 C -0.193168 0.017299

39 C -0.212426 -0.006634

40 C -0.209418 0.016595

41 C -0.212352 -0.006939

42 C -0.195786 0.017384

43 C -0.138257 -0.019788

44 C -0.193168 0.017299

45 C -0.212426 -0.006634

46 C -0.209418 0.016595

47 C -0.212352 -0.006939

48 C -0.195786 0.017384

49 H 0.267980 -0.000245

50 H 0.267980 -0.000245

51 H 0.252780 0.000668

52 H 0.252780 0.000668

53 H 0.252780 0.000668

54 H 0.252780 0.000668

55 H 0.267980 -0.000245

56 H 0.267980 -0.000245

57 H 0.235182 -0.000836

58 H 0.232767 0.000661

59 H 0.232665 -0.000861

60 H 0.232815 0.000657

61 H 0.234393 -0.000721

62 H 0.232665 -0.000861

63 H 0.232767 0.000661

64 H 0.235182 -0.000836

65 H 0.234393 -0.000721

66 H 0.232815 0.000657

67 H 0.234393 -0.000721

68 H 0.232815 0.000657

69 H 0.232665 -0.000861

70 H 0.232767 0.000661

71 H 0.235182 -0.000836

72 H 0.234393 -0.000721

73 H 0.232815 0.000657

74 H 0.232665 -0.000861

75 H 0.232767 0.000661

76 H 0.235182 -0.000836

77 H 0.437565 -0.003371

78 H 0.437565 -0.003371

Sum of Mulliken charges = 1.00000 1.00000

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

1 2

1 C 0.035114 0.011024

2 C 0.375669 -0.045380

3 N -0.258785 0.067791

4 C 0.375669 -0.045380

5 C 0.035114 0.011024

6 C -0.058506 0.240844

7 C 0.241049 -0.078041

8 N -0.484908 0.160011

9 C 0.241049 -0.078041

10 C 0.022108 -0.009166

11 C 0.022108 -0.009166

12 C -0.058506 0.240844

13 C 0.241049 -0.078041

14 C 0.022108 -0.009166

15 C 0.022108 -0.009166

16 C 0.241049 -0.078041

17 N -0.484908 0.160011

18 C -0.058506 0.240844

19 C 0.375669 -0.045380

20 C 0.035114 0.011024

21 C 0.035114 0.011024

22 C 0.375669 -0.045380

23 N -0.258785 0.067791

24 C -0.058506 0.240844

25 C -0.138257 -0.019788

26 C 0.039396 0.016549

27 C 0.020415 -0.006279

28 C 0.023246 0.015734

29 C 0.020389 -0.005977

30 C 0.041225 0.016578

31 C 0.023246 0.015734

32 C 0.020415 -0.006279

33 C 0.039396 0.016549

34 C -0.138257 -0.019788

35 C 0.041225 0.016578

36 C 0.020389 -0.005977

37 C -0.138257 -0.019788

38 C 0.041225 0.016578

39 C 0.020389 -0.005977

40 C 0.023246 0.015734

41 C 0.020415 -0.006279

42 C 0.039396 0.016549

43 C -0.138257 -0.019788

44 C 0.041225 0.016578

45 C 0.020389 -0.005977

46 C 0.023246 0.015734

47 C 0.020415 -0.006279

48 C 0.039396 0.016549

Electronic spatial extent (au): <R\*\*2>= 33105.2634

Charge= 1.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 0.0000 Y= -0.0000 Z= -0.2576 Tot= 0.2576

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

XX= -178.4493 YY= -160.2686 ZZ= -261.6938

XY= -0.0000 XZ= -0.0000 YZ= 0.0000

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

XX= 21.6880 YY= 39.8686 ZZ= -61.5566

XY= -0.0000 XZ= -0.0000 YZ= 0.0000

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

XXX= -0.0000 YYY= -0.0000 ZZZ= 1.2475 XYY= -0.0000

XXY= -0.0000 XXZ= 94.6666 XZZ= 0.0000 YZZ= -0.0000

YYZ= -91.6951 XYZ= 0.0000

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

XXXX= -20074.3989 YYYY= -19421.8884 ZZZZ= -1046.9506 XXXY= -0.0000

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

ZZZY= 0.0000 XXYY= -4688.2505 XXZZ= -3730.5132 YYZZ= -3679.1555

XXYZ= 0.0000 YYXZ= -0.0000 ZZXY= 0.0000

N-N= 5.358814831867D+03 E-N=-1.513182194563D+04 KE= 1.906089589401D+03

Symmetry A1 KE= 5.306495201667D+02

Symmetry A2 KE= 4.229898456043D+02

Symmetry B1 KE= 4.763151053409D+02

Symmetry B2 KE= 4.761351182890D+02

Isotropic Fermi Contact Couplings

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

1 C(13) 0.00054 0.61201 0.21838 0.20414

2 C(13) -0.01051 -11.81739 -4.21674 -3.94186

3 N(14) 0.00844 2.72818 0.97348 0.91002

4 C(13) -0.01051 -11.81739 -4.21674 -3.94186

5 C(13) 0.00054 0.61201 0.21838 0.20414

6 C(13) 0.01453 16.33638 5.82922 5.44923

7 C(13) -0.01362 -15.30641 -5.46171 -5.10567

8 N(14) 0.01535 4.95844 1.76930 1.65396

9 C(13) -0.01362 -15.30641 -5.46171 -5.10567

10 C(13) 0.00037 0.41449 0.14790 0.13826

11 C(13) 0.00037 0.41449 0.14790 0.13826

12 C(13) 0.01453 16.33638 5.82922 5.44923

13 C(13) -0.01362 -15.30641 -5.46171 -5.10567

14 C(13) 0.00037 0.41449 0.14790 0.13826

15 C(13) 0.00037 0.41449 0.14790 0.13826

16 C(13) -0.01362 -15.30641 -5.46171 -5.10567

17 N(14) 0.01535 4.95844 1.76930 1.65396

18 C(13) 0.01453 16.33638 5.82922 5.44923

19 C(13) -0.01051 -11.81739 -4.21674 -3.94186

20 C(13) 0.00054 0.61201 0.21838 0.20414

21 C(13) 0.00054 0.61201 0.21838 0.20414

22 C(13) -0.01051 -11.81739 -4.21674 -3.94186

23 N(14) 0.00844 2.72818 0.97348 0.91002

24 C(13) 0.01453 16.33638 5.82922 5.44923

25 C(13) -0.00758 -8.52642 -3.04244 -2.84411

26 C(13) 0.00788 8.86247 3.16235 2.95620

27 C(13) -0.00008 -0.08799 -0.03140 -0.02935

28 C(13) 0.00097 1.08512 0.38720 0.36196

29 C(13) -0.00001 -0.01169 -0.00417 -0.00390

30 C(13) 0.00825 9.27701 3.31027 3.09448

31 C(13) 0.00097 1.08512 0.38720 0.36196

32 C(13) -0.00008 -0.08799 -0.03140 -0.02935

33 C(13) 0.00788 8.86247 3.16235 2.95620

34 C(13) -0.00758 -8.52642 -3.04244 -2.84411

35 C(13) 0.00825 9.27701 3.31027 3.09448

36 C(13) -0.00001 -0.01169 -0.00417 -0.00390

37 C(13) -0.00758 -8.52642 -3.04244 -2.84411

38 C(13) 0.00825 9.27701 3.31027 3.09448

39 C(13) -0.00001 -0.01169 -0.00417 -0.00390

40 C(13) 0.00097 1.08512 0.38720 0.36196

41 C(13) -0.00008 -0.08799 -0.03140 -0.02935

42 C(13) 0.00788 8.86247 3.16235 2.95620

43 C(13) -0.00758 -8.52642 -3.04244 -2.84411

44 C(13) 0.00825 9.27701 3.31027 3.09448

45 C(13) -0.00001 -0.01169 -0.00417 -0.00390

46 C(13) 0.00097 1.08512 0.38720 0.36196

47 C(13) -0.00008 -0.08799 -0.03140 -0.02935

48 C(13) 0.00788 8.86247 3.16235 2.95620

49 H(1) -0.00011 -0.51284 -0.18300 -0.17107

50 H(1) -0.00011 -0.51284 -0.18300 -0.17107

51 H(1) 0.00020 0.88022 0.31409 0.29361

52 H(1) 0.00020 0.88022 0.31409 0.29361

53 H(1) 0.00020 0.88022 0.31409 0.29361

54 H(1) 0.00020 0.88022 0.31409 0.29361

55 H(1) -0.00011 -0.51284 -0.18300 -0.17107

56 H(1) -0.00011 -0.51284 -0.18300 -0.17107

57 H(1) -0.00029 -1.31069 -0.46769 -0.43720

58 H(1) 0.00023 1.03428 0.36906 0.34500

59 H(1) -0.00023 -1.04582 -0.37317 -0.34885

60 H(1) 0.00023 1.04670 0.37349 0.34914

61 H(1) -0.00029 -1.29029 -0.46041 -0.43039

62 H(1) -0.00023 -1.04582 -0.37317 -0.34885

63 H(1) 0.00023 1.03428 0.36906 0.34500

64 H(1) -0.00029 -1.31069 -0.46769 -0.43720

65 H(1) -0.00029 -1.29029 -0.46041 -0.43039

66 H(1) 0.00023 1.04670 0.37349 0.34914

67 H(1) -0.00029 -1.29029 -0.46041 -0.43039

68 H(1) 0.00023 1.04670 0.37349 0.34914

69 H(1) -0.00023 -1.04582 -0.37317 -0.34885

70 H(1) 0.00023 1.03428 0.36906 0.34500

71 H(1) -0.00029 -1.31069 -0.46769 -0.43720

72 H(1) -0.00029 -1.29029 -0.46041 -0.43039

73 H(1) 0.00023 1.04670 0.37349 0.34914

74 H(1) -0.00023 -1.04582 -0.37317 -0.34885

75 H(1) 0.00023 1.03428 0.36906 0.34500

76 H(1) -0.00029 -1.31069 -0.46769 -0.43720

77 H(1) -0.00108 -4.82846 -1.72292 -1.61060

78 H(1) -0.00108 -4.82846 -1.72292 -1.61060

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

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

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

1 Atom -0.003571 -0.003182 0.006753

2 Atom 0.025028 0.012311 -0.037340

3 Atom -0.078790 -0.083092 0.161882

4 Atom 0.025028 0.012311 -0.037340

5 Atom -0.003571 -0.003182 0.006753

6 Atom -0.134333 -0.134478 0.268811

7 Atom 0.028960 0.044570 -0.073530

8 Atom -0.177422 -0.177274 0.354695

9 Atom 0.028960 0.044570 -0.073530

10 Atom 0.010008 0.007821 -0.017829

11 Atom 0.010008 0.007821 -0.017829

12 Atom -0.134333 -0.134478 0.268811

13 Atom 0.028960 0.044570 -0.073530

14 Atom 0.010008 0.007821 -0.017829

15 Atom 0.010008 0.007821 -0.017829

16 Atom 0.028960 0.044570 -0.073530

17 Atom -0.177422 -0.177274 0.354695

18 Atom -0.134333 -0.134478 0.268811

19 Atom 0.025028 0.012311 -0.037340

20 Atom -0.003571 -0.003182 0.006753

21 Atom -0.003571 -0.003182 0.006753

22 Atom 0.025028 0.012311 -0.037340

23 Atom -0.078790 -0.083092 0.161882

24 Atom -0.134333 -0.134478 0.268811

25 Atom -0.002923 -0.003583 0.006506

26 Atom -0.006773 0.016981 -0.010208

27 Atom -0.001201 0.001586 -0.000384

28 Atom 0.001631 0.001591 -0.003222

29 Atom 0.002115 -0.001573 -0.000542

30 Atom 0.017144 -0.007153 -0.009991

31 Atom 0.001631 0.001591 -0.003222

32 Atom -0.001201 0.001586 -0.000384

33 Atom -0.006773 0.016981 -0.010208

34 Atom -0.002923 -0.003583 0.006506

35 Atom 0.017144 -0.007153 -0.009991

36 Atom 0.002115 -0.001573 -0.000542

37 Atom -0.002923 -0.003583 0.006506

38 Atom 0.017144 -0.007153 -0.009991

39 Atom 0.002115 -0.001573 -0.000542

40 Atom 0.001631 0.001591 -0.003222

41 Atom -0.001201 0.001586 -0.000384

42 Atom -0.006773 0.016981 -0.010208

43 Atom -0.002923 -0.003583 0.006506

44 Atom 0.017144 -0.007153 -0.009991

45 Atom 0.002115 -0.001573 -0.000542

46 Atom 0.001631 0.001591 -0.003222

47 Atom -0.001201 0.001586 -0.000384

48 Atom -0.006773 0.016981 -0.010208

49 Atom 0.000331 0.001285 -0.001616

50 Atom 0.000331 0.001285 -0.001616

51 Atom 0.001323 -0.000060 -0.001262

52 Atom 0.001323 -0.000060 -0.001262

53 Atom 0.001323 -0.000060 -0.001262

54 Atom 0.001323 -0.000060 -0.001262

55 Atom 0.000331 0.001285 -0.001616

56 Atom 0.000331 0.001285 -0.001616

57 Atom -0.000753 0.000353 0.000400

58 Atom -0.000015 0.000197 -0.000182

59 Atom 0.000645 0.000566 -0.001211

60 Atom 0.000263 -0.000111 -0.000152

61 Atom 0.000508 -0.000853 0.000345

62 Atom 0.000645 0.000566 -0.001211

63 Atom -0.000015 0.000197 -0.000182

64 Atom -0.000753 0.000353 0.000400

65 Atom 0.000508 -0.000853 0.000345

66 Atom 0.000263 -0.000111 -0.000152

67 Atom 0.000508 -0.000853 0.000345

68 Atom 0.000263 -0.000111 -0.000152

69 Atom 0.000645 0.000566 -0.001211

70 Atom -0.000015 0.000197 -0.000182

71 Atom -0.000753 0.000353 0.000400

72 Atom 0.000508 -0.000853 0.000345

73 Atom 0.000263 -0.000111 -0.000152

74 Atom 0.000645 0.000566 -0.001211

75 Atom -0.000015 0.000197 -0.000182

76 Atom -0.000753 0.000353 0.000400

77 Atom -0.001666 0.007608 -0.005942

78 Atom -0.001666 0.007608 -0.005942

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XY XZ YZ

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

1 Atom 0.000781 0.001167 -0.003492

2 Atom 0.001565 -0.001850 0.003322

3 Atom -0.000000 0.000000 -0.027560

4 Atom -0.001565 0.001850 0.003322

5 Atom -0.000781 -0.001167 -0.003492

6 Atom 0.002594 0.009394 -0.011890

7 Atom 0.003851 -0.010291 0.000089

8 Atom 0.000000 0.061376 -0.000000

9 Atom -0.003851 -0.010291 -0.000089

10 Atom 0.000325 -0.002754 -0.000007

11 Atom -0.000325 -0.002754 0.000007

12 Atom -0.002594 -0.009394 -0.011890

13 Atom -0.003851 0.010291 0.000089

14 Atom 0.000325 0.002754 0.000007

15 Atom -0.000325 0.002754 -0.000007

16 Atom 0.003851 0.010291 -0.000089

17 Atom -0.000000 -0.061376 0.000000

18 Atom 0.002594 -0.009394 0.011890

19 Atom -0.001565 -0.001850 -0.003322

20 Atom -0.000781 0.001167 0.003492

21 Atom 0.000781 -0.001167 0.003492

22 Atom 0.001565 0.001850 -0.003322

23 Atom 0.000000 -0.000000 0.027560

24 Atom -0.002594 0.009394 0.011890

25 Atom 0.007347 0.001862 -0.001669

26 Atom -0.007657 -0.002348 0.000253

27 Atom 0.005655 0.003055 -0.003077

28 Atom -0.009113 -0.008037 0.008076

29 Atom 0.005453 0.002978 -0.003088

30 Atom -0.007552 0.000200 0.002049

31 Atom 0.009113 0.008037 0.008076

32 Atom -0.005655 -0.003055 -0.003077

33 Atom 0.007657 0.002348 0.000253

34 Atom -0.007347 -0.001862 -0.001669

35 Atom 0.007552 -0.000200 0.002049

36 Atom -0.005453 -0.002978 -0.003088

37 Atom -0.007347 0.001862 0.001669

38 Atom 0.007552 0.000200 -0.002049

39 Atom -0.005453 0.002978 0.003088

40 Atom 0.009113 -0.008037 -0.008076

41 Atom -0.005655 0.003055 0.003077

42 Atom 0.007657 -0.002348 -0.000253

43 Atom 0.007347 -0.001862 0.001669

44 Atom -0.007552 -0.000200 -0.002049

45 Atom 0.005453 -0.002978 0.003088

46 Atom -0.009113 0.008037 -0.008076

47 Atom 0.005655 -0.003055 0.003077

48 Atom -0.007657 0.002348 -0.000253

49 Atom -0.000139 -0.000143 0.000353

50 Atom 0.000139 0.000143 0.000353

51 Atom 0.001564 -0.000245 -0.000235

52 Atom -0.001564 -0.000245 0.000235

53 Atom 0.001564 0.000245 0.000235

54 Atom -0.001564 0.000245 -0.000235

55 Atom 0.000139 -0.000143 -0.000353

56 Atom -0.000139 0.000143 -0.000353

57 Atom 0.000555 0.000606 -0.002356

58 Atom 0.000703 -0.000002 -0.000250

59 Atom 0.001187 -0.000251 0.000276

60 Atom 0.000665 0.000270 -0.000028

61 Atom 0.000412 0.002371 -0.000920

62 Atom -0.001187 0.000251 0.000276

63 Atom -0.000703 0.000002 -0.000250

64 Atom -0.000555 -0.000606 -0.002356

65 Atom -0.000412 -0.002371 -0.000920

66 Atom -0.000665 -0.000270 -0.000028

67 Atom -0.000412 0.002371 0.000920

68 Atom -0.000665 0.000270 0.000028

69 Atom -0.001187 -0.000251 -0.000276

70 Atom -0.000703 -0.000002 0.000250

71 Atom -0.000555 0.000606 0.002356

72 Atom 0.000412 -0.002371 0.000920

73 Atom 0.000665 -0.000270 0.000028

74 Atom 0.001187 0.000251 -0.000276

75 Atom 0.000703 0.000002 0.000250

76 Atom 0.000555 -0.000606 0.002356

77 Atom -0.000000 -0.000000 0.001402

78 Atom 0.000000 0.000000 -0.001402

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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 -0.0051 -0.685 -0.244 -0.228 -0.5967 0.7520 0.2802

1 C(13) Bbb -0.0028 -0.379 -0.135 -0.126 0.7988 0.5899 0.1178

Bcc 0.0079 1.064 0.379 0.355 0.0767 -0.2941 0.9527

Baa -0.0376 -5.049 -1.801 -1.684 0.0311 -0.0673 0.9972

2 C(13) Bbb 0.0124 1.660 0.592 0.554 -0.1122 0.9912 0.0704

Bcc 0.0253 3.389 1.209 1.130 0.9932 0.1141 -0.0233

Baa -0.0862 -3.323 -1.186 -1.108 -0.0000 0.9939 0.1104

3 N(14) Bbb -0.0788 -3.039 -1.084 -1.014 1.0000 0.0000 0.0000

Bcc 0.1649 6.362 2.270 2.122 0.0000 -0.1104 0.9939

Baa -0.0376 -5.049 -1.801 -1.684 -0.0311 -0.0673 0.9972

4 C(13) Bbb 0.0124 1.660 0.592 0.554 0.1122 0.9912 0.0704

Bcc 0.0253 3.389 1.209 1.130 0.9932 -0.1141 0.0233

Baa -0.0051 -0.685 -0.244 -0.228 0.5967 0.7520 0.2802

5 C(13) Bbb -0.0028 -0.379 -0.135 -0.126 0.7988 -0.5899 -0.1178

Bcc 0.0079 1.064 0.379 0.355 -0.0767 -0.2941 0.9527

Baa -0.1376 -18.459 -6.587 -6.157 -0.6894 0.7234 0.0371

6 C(13) Bbb -0.1318 -17.688 -6.312 -5.900 0.7240 0.6898 0.0035

Bcc 0.2694 36.148 12.898 12.058 0.0231 -0.0293 0.9993

Baa -0.0746 -10.005 -3.570 -3.337 0.0991 -0.0039 0.9951

7 C(13) Bbb 0.0290 3.897 1.391 1.300 0.9661 -0.2390 -0.0971

Bcc 0.0455 6.107 2.179 2.037 0.2382 0.9710 -0.0199

Baa -0.1844 -7.112 -2.538 -2.372 0.9936 -0.0000 -0.1131

8 N(14) Bbb -0.1773 -6.837 -2.440 -2.281 0.0000 1.0000 -0.0000

Bcc 0.3617 13.949 4.977 4.653 0.1131 -0.0000 0.9936

Baa -0.0746 -10.005 -3.570 -3.337 0.0991 0.0039 0.9951

9 C(13) Bbb 0.0290 3.897 1.391 1.300 0.9661 0.2390 -0.0971

Bcc 0.0455 6.107 2.179 2.037 -0.2382 0.9710 0.0199

Baa -0.0181 -2.429 -0.867 -0.810 0.0975 -0.0009 0.9952

10 C(13) Bbb 0.0078 1.044 0.373 0.348 -0.1279 0.9917 0.0135

Bcc 0.0103 1.385 0.494 0.462 0.9870 0.1286 -0.0966

Baa -0.0181 -2.429 -0.867 -0.810 0.0975 0.0009 0.9952

11 C(13) Bbb 0.0078 1.044 0.373 0.348 0.1279 0.9917 -0.0135

Bcc 0.0103 1.385 0.494 0.462 0.9870 -0.1286 -0.0966

Baa -0.1376 -18.459 -6.587 -6.157 0.6894 0.7234 0.0371

12 C(13) Bbb -0.1318 -17.688 -6.312 -5.900 0.7240 -0.6898 -0.0035

Bcc 0.2694 36.148 12.898 12.058 -0.0231 -0.0293 0.9993

Baa -0.0746 -10.005 -3.570 -3.337 -0.0991 -0.0039 0.9951

13 C(13) Bbb 0.0290 3.897 1.391 1.300 0.9661 0.2390 0.0971

Bcc 0.0455 6.107 2.179 2.037 -0.2382 0.9710 -0.0199

Baa -0.0181 -2.429 -0.867 -0.810 -0.0975 0.0009 0.9952

14 C(13) Bbb 0.0078 1.044 0.373 0.348 -0.1279 0.9917 -0.0135

Bcc 0.0103 1.385 0.494 0.462 0.9870 0.1286 0.0966

Baa -0.0181 -2.429 -0.867 -0.810 -0.0975 -0.0009 0.9952

15 C(13) Bbb 0.0078 1.044 0.373 0.348 0.1279 0.9917 0.0135

Bcc 0.0103 1.385 0.494 0.462 0.9870 -0.1286 0.0966

Baa -0.0746 -10.005 -3.570 -3.337 -0.0991 0.0039 0.9951

16 C(13) Bbb 0.0290 3.897 1.391 1.300 0.9661 -0.2390 0.0971

Bcc 0.0455 6.107 2.179 2.037 0.2382 0.9710 0.0199

Baa -0.1844 -7.112 -2.538 -2.372 0.9936 0.0000 0.1131

17 N(14) Bbb -0.1773 -6.837 -2.440 -2.281 -0.0000 1.0000 -0.0000

Bcc 0.3617 13.949 4.977 4.653 -0.1131 0.0000 0.9936

Baa -0.1376 -18.459 -6.587 -6.157 -0.6894 0.7234 -0.0371

18 C(13) Bbb -0.1318 -17.688 -6.312 -5.900 0.7240 0.6898 -0.0035

Bcc 0.2694 36.148 12.898 12.058 -0.0231 0.0293 0.9993

Baa -0.0376 -5.049 -1.801 -1.684 0.0311 0.0673 0.9972

19 C(13) Bbb 0.0124 1.660 0.592 0.554 0.1122 0.9912 -0.0704

Bcc 0.0253 3.389 1.209 1.130 0.9932 -0.1141 -0.0233

Baa -0.0051 -0.685 -0.244 -0.228 0.5967 0.7520 -0.2802

20 C(13) Bbb -0.0028 -0.379 -0.135 -0.126 0.7988 -0.5899 0.1178

Bcc 0.0079 1.064 0.379 0.355 0.0767 0.2941 0.9527

Baa -0.0051 -0.685 -0.244 -0.228 -0.5967 0.7520 -0.2802

21 C(13) Bbb -0.0028 -0.379 -0.135 -0.126 0.7988 0.5899 -0.1178

Bcc 0.0079 1.064 0.379 0.355 -0.0767 0.2941 0.9527

Baa -0.0376 -5.049 -1.801 -1.684 -0.0311 0.0673 0.9972

22 C(13) Bbb 0.0124 1.660 0.592 0.554 -0.1122 0.9912 -0.0704

Bcc 0.0253 3.389 1.209 1.130 0.9932 0.1141 0.0233

Baa -0.0862 -3.323 -1.186 -1.108 -0.0000 0.9939 -0.1104

23 N(14) Bbb -0.0788 -3.039 -1.084 -1.014 1.0000 0.0000 -0.0000

Bcc 0.1649 6.362 2.270 2.122 -0.0000 0.1104 0.9939

Baa -0.1376 -18.459 -6.587 -6.157 0.6894 0.7234 -0.0371

24 C(13) Bbb -0.1318 -17.688 -6.312 -5.900 0.7240 -0.6898 0.0035

Bcc 0.2694 36.148 12.898 12.058 0.0231 0.0293 0.9993

Baa -0.0110 -1.471 -0.525 -0.491 -0.6854 0.7143 0.1413

25 C(13) Bbb 0.0041 0.549 0.196 0.183 0.7132 0.6977 -0.0676

Bcc 0.0069 0.923 0.329 0.308 0.1469 -0.0545 0.9877

Baa -0.0119 -1.596 -0.569 -0.532 0.5872 0.1487 0.7957

26 C(13) Bbb -0.0074 -0.989 -0.353 -0.330 0.7578 0.2446 -0.6050

Bcc 0.0193 2.585 0.922 0.862 -0.2846 0.9582 0.0309

Baa -0.0081 -1.081 -0.386 -0.360 0.6744 -0.5522 -0.4902

27 C(13) Bbb 0.0020 0.265 0.095 0.088 0.4559 -0.2109 0.8647

Bcc 0.0061 0.815 0.291 0.272 0.5809 0.8066 -0.1095

Baa -0.0096 -1.289 -0.460 -0.430 0.3343 -0.3570 0.8723

28 C(13) Bbb -0.0075 -1.007 -0.359 -0.336 0.7125 0.7016 0.0141

Bcc 0.0171 2.296 0.819 0.766 0.6170 -0.6167 -0.4889

Baa -0.0079 -1.065 -0.380 -0.355 -0.5229 0.6908 0.4994

29 C(13) Bbb 0.0018 0.246 0.088 0.082 0.1874 -0.4783 0.8580

Bcc 0.0061 0.819 0.292 0.273 0.8315 0.5422 0.1207

Baa -0.0117 -1.571 -0.561 -0.524 -0.1684 -0.6230 0.7638

30 C(13) Bbb -0.0076 -1.020 -0.364 -0.340 0.2182 0.7321 0.6453

Bcc 0.0193 2.591 0.924 0.864 0.9613 -0.2754 -0.0127

Baa -0.0096 -1.289 -0.460 -0.430 -0.3343 -0.3570 0.8723

31 C(13) Bbb -0.0075 -1.007 -0.359 -0.336 0.7125 -0.7016 -0.0141

Bcc 0.0171 2.296 0.819 0.766 0.6170 0.6167 0.4889

Baa -0.0081 -1.081 -0.386 -0.360 0.6744 0.5522 0.4902

32 C(13) Bbb 0.0020 0.265 0.095 0.088 -0.4559 -0.2109 0.8647

Bcc 0.0061 0.815 0.291 0.272 -0.5809 0.8066 -0.1095

Baa -0.0119 -1.596 -0.569 -0.532 -0.5872 0.1487 0.7957

33 C(13) Bbb -0.0074 -0.989 -0.353 -0.330 0.7578 -0.2446 0.6050

Bcc 0.0193 2.585 0.922 0.862 0.2846 0.9582 0.0309

Baa -0.0110 -1.471 -0.525 -0.491 0.6854 0.7143 0.1413

34 C(13) Bbb 0.0041 0.549 0.196 0.183 0.7132 -0.6977 0.0676

Bcc 0.0069 0.923 0.329 0.308 -0.1469 -0.0545 0.9877

Baa -0.0117 -1.571 -0.561 -0.524 0.1684 -0.6230 0.7638

35 C(13) Bbb -0.0076 -1.020 -0.364 -0.340 -0.2182 0.7321 0.6453

Bcc 0.0193 2.591 0.924 0.864 0.9613 0.2754 0.0127

Baa -0.0079 -1.065 -0.380 -0.355 0.5229 0.6908 0.4994

36 C(13) Bbb 0.0018 0.246 0.088 0.082 -0.1874 -0.4783 0.8580

Bcc 0.0061 0.819 0.292 0.273 0.8315 -0.5422 -0.1207

Baa -0.0110 -1.471 -0.525 -0.491 0.6854 0.7143 -0.1413

37 C(13) Bbb 0.0041 0.549 0.196 0.183 0.7132 -0.6977 -0.0676

Bcc 0.0069 0.923 0.329 0.308 0.1469 0.0545 0.9877

Baa -0.0117 -1.571 -0.561 -0.524 -0.1684 0.6230 0.7638

38 C(13) Bbb -0.0076 -1.020 -0.364 -0.340 -0.2182 0.7321 -0.6453

Bcc 0.0193 2.591 0.924 0.864 0.9613 0.2754 -0.0127

Baa -0.0079 -1.065 -0.380 -0.355 0.5229 0.6908 -0.4994

39 C(13) Bbb 0.0018 0.246 0.088 0.082 0.1874 0.4783 0.8580

Bcc 0.0061 0.819 0.292 0.273 0.8315 -0.5422 0.1207

Baa -0.0096 -1.289 -0.460 -0.430 0.3343 0.3570 0.8723

40 C(13) Bbb -0.0075 -1.007 -0.359 -0.336 0.7125 -0.7016 0.0141

Bcc 0.0171 2.296 0.819 0.766 0.6170 0.6167 -0.4889

Baa -0.0081 -1.081 -0.386 -0.360 0.6744 0.5522 -0.4902

41 C(13) Bbb 0.0020 0.265 0.095 0.088 0.4559 0.2109 0.8647

Bcc 0.0061 0.815 0.291 0.272 -0.5809 0.8066 0.1095

Baa -0.0119 -1.596 -0.569 -0.532 0.5872 -0.1487 0.7957

42 C(13) Bbb -0.0074 -0.989 -0.353 -0.330 0.7578 -0.2446 -0.6050

Bcc 0.0193 2.585 0.922 0.862 0.2846 0.9582 -0.0309

Baa -0.0110 -1.471 -0.525 -0.491 -0.6854 0.7143 -0.1413

43 C(13) Bbb 0.0041 0.549 0.196 0.183 0.7132 0.6977 0.0676

Bcc 0.0069 0.923 0.329 0.308 -0.1469 0.0545 0.9877

Baa -0.0117 -1.571 -0.561 -0.524 0.1684 0.6230 0.7638

44 C(13) Bbb -0.0076 -1.020 -0.364 -0.340 0.2182 0.7321 -0.6453

Bcc 0.0193 2.591 0.924 0.864 0.9613 -0.2754 0.0127

Baa -0.0079 -1.065 -0.380 -0.355 -0.5229 0.6908 -0.4994

45 C(13) Bbb 0.0018 0.246 0.088 0.082 -0.1874 0.4783 0.8580

Bcc 0.0061 0.819 0.292 0.273 0.8315 0.5422 -0.1207

Baa -0.0096 -1.289 -0.460 -0.430 -0.3343 0.3570 0.8723

46 C(13) Bbb -0.0075 -1.007 -0.359 -0.336 0.7125 0.7016 -0.0141

Bcc 0.0171 2.296 0.819 0.766 0.6170 -0.6167 0.4889

Baa -0.0081 -1.081 -0.386 -0.360 0.6744 -0.5522 0.4902

47 C(13) Bbb 0.0020 0.265 0.095 0.088 -0.4559 0.2109 0.8647

Bcc 0.0061 0.815 0.291 0.272 0.5809 0.8066 0.1095

Baa -0.0119 -1.596 -0.569 -0.532 -0.5872 -0.1487 0.7957

48 C(13) Bbb -0.0074 -0.989 -0.353 -0.330 0.7578 0.2446 0.6050

Bcc 0.0193 2.585 0.922 0.862 -0.2846 0.9582 -0.0309

Baa -0.0017 -0.889 -0.317 -0.297 0.0629 -0.1157 0.9913

49 H(1) Bbb 0.0003 0.168 0.060 0.056 0.9865 0.1578 -0.0442

Bcc 0.0014 0.721 0.257 0.241 -0.1513 0.9807 0.1240

Baa -0.0017 -0.889 -0.317 -0.297 -0.0629 -0.1157 0.9913

50 H(1) Bbb 0.0003 0.168 0.060 0.056 0.9865 -0.1578 0.0442

Bcc 0.0014 0.721 0.257 0.241 0.1513 0.9807 0.1240

Baa -0.0013 -0.699 -0.249 -0.233 -0.0689 0.2669 0.9613

51 H(1) Bbb -0.0011 -0.566 -0.202 -0.189 -0.5481 0.7950 -0.2600

Bcc 0.0024 1.265 0.452 0.422 0.8336 0.5448 -0.0915

Baa -0.0013 -0.699 -0.249 -0.233 -0.0689 -0.2669 0.9613

52 H(1) Bbb -0.0011 -0.566 -0.202 -0.189 0.5481 0.7950 0.2600

Bcc 0.0024 1.265 0.452 0.422 0.8336 -0.5448 -0.0915

Baa -0.0013 -0.699 -0.249 -0.233 0.0689 -0.2669 0.9613

53 H(1) Bbb -0.0011 -0.566 -0.202 -0.189 -0.5481 0.7950 0.2600

Bcc 0.0024 1.265 0.452 0.422 0.8336 0.5448 0.0915

Baa -0.0013 -0.699 -0.249 -0.233 0.0689 0.2669 0.9613

54 H(1) Bbb -0.0011 -0.566 -0.202 -0.189 0.5481 0.7950 -0.2600

Bcc 0.0024 1.265 0.452 0.422 0.8336 -0.5448 0.0915

Baa -0.0017 -0.889 -0.317 -0.297 0.0629 0.1157 0.9913

55 H(1) Bbb 0.0003 0.168 0.060 0.056 0.9865 -0.1578 -0.0442

Bcc 0.0014 0.721 0.257 0.241 0.1513 0.9807 -0.1240

Baa -0.0017 -0.889 -0.317 -0.297 -0.0629 0.1157 0.9913

56 H(1) Bbb 0.0003 0.168 0.060 0.056 0.9865 0.1578 0.0442

Bcc 0.0014 0.721 0.257 0.241 -0.1513 0.9807 -0.1240

Baa -0.0024 -1.276 -0.455 -0.426 -0.4482 0.6327 0.6315

57 H(1) Bbb -0.0003 -0.182 -0.065 -0.061 0.8938 0.3267 0.3071

Bcc 0.0027 1.458 0.520 0.486 0.0120 -0.7021 0.7120

Baa -0.0007 -0.360 -0.128 -0.120 0.6887 -0.6480 -0.3254

58 H(1) Bbb -0.0002 -0.087 -0.031 -0.029 0.3676 -0.0748 0.9270

Bcc 0.0008 0.447 0.160 0.149 0.6250 0.7580 -0.1867

Baa -0.0014 -0.739 -0.264 -0.246 0.2905 -0.3050 0.9070

59 H(1) Bbb -0.0004 -0.218 -0.078 -0.073 -0.6322 0.6503 0.4212

Bcc 0.0018 0.957 0.341 0.319 0.7183 0.6958 0.0039

Baa -0.0007 -0.365 -0.130 -0.122 -0.6037 0.7189 0.3444

60 H(1) Bbb -0.0001 -0.067 -0.024 -0.022 0.0466 -0.3995 0.9156

Bcc 0.0008 0.432 0.154 0.144 0.7958 0.5688 0.2077

Baa -0.0025 -1.334 -0.476 -0.445 -0.5764 0.5038 0.6434

61 H(1) Bbb -0.0003 -0.178 -0.063 -0.059 0.4181 0.8583 -0.2975

Bcc 0.0028 1.511 0.539 0.504 0.7021 -0.0975 0.7054

Baa -0.0014 -0.739 -0.264 -0.246 -0.2905 -0.3050 0.9070

62 H(1) Bbb -0.0004 -0.218 -0.078 -0.073 0.6322 0.6503 0.4212

Bcc 0.0018 0.957 0.341 0.319 0.7183 -0.6958 -0.0039

Baa -0.0007 -0.360 -0.128 -0.120 0.6887 0.6480 0.3254

63 H(1) Bbb -0.0002 -0.087 -0.031 -0.029 -0.3676 -0.0748 0.9270

Bcc 0.0008 0.447 0.160 0.149 -0.6250 0.7580 -0.1867

Baa -0.0024 -1.276 -0.455 -0.426 0.4482 0.6327 0.6315

64 H(1) Bbb -0.0003 -0.182 -0.065 -0.061 0.8938 -0.3267 -0.3071

Bcc 0.0027 1.458 0.520 0.486 -0.0120 -0.7021 0.7120

Baa -0.0025 -1.334 -0.476 -0.445 0.5764 0.5038 0.6434

65 H(1) Bbb -0.0003 -0.178 -0.063 -0.059 -0.4181 0.8583 -0.2975

Bcc 0.0028 1.511 0.539 0.504 -0.7021 -0.0975 0.7054

Baa -0.0007 -0.365 -0.130 -0.122 0.6037 0.7189 0.3444

66 H(1) Bbb -0.0001 -0.067 -0.024 -0.022 -0.0466 -0.3995 0.9156

Bcc 0.0008 0.432 0.154 0.144 0.7958 -0.5688 -0.2077

Baa -0.0025 -1.334 -0.476 -0.445 -0.5764 -0.5038 0.6434

67 H(1) Bbb -0.0003 -0.178 -0.063 -0.059 -0.4181 0.8583 0.2975

Bcc 0.0028 1.511 0.539 0.504 0.7021 0.0975 0.7054

Baa -0.0007 -0.365 -0.130 -0.122 0.6037 0.7189 -0.3444

68 H(1) Bbb -0.0001 -0.067 -0.024 -0.022 0.0466 0.3995 0.9156

Bcc 0.0008 0.432 0.154 0.144 0.7958 -0.5688 0.2077

Baa -0.0014 -0.739 -0.264 -0.246 0.2905 0.3050 0.9070

69 H(1) Bbb -0.0004 -0.218 -0.078 -0.073 0.6322 0.6503 -0.4212

Bcc 0.0018 0.957 0.341 0.319 0.7183 -0.6958 0.0039

Baa -0.0007 -0.360 -0.128 -0.120 0.6887 0.6480 -0.3254

70 H(1) Bbb -0.0002 -0.087 -0.031 -0.029 0.3676 0.0748 0.9270

Bcc 0.0008 0.447 0.160 0.149 -0.6250 0.7580 0.1867

Baa -0.0024 -1.276 -0.455 -0.426 0.4482 0.6327 -0.6315

71 H(1) Bbb -0.0003 -0.182 -0.065 -0.061 0.8938 -0.3267 0.3071

Bcc 0.0027 1.458 0.520 0.486 0.0120 0.7021 0.7120

Baa -0.0025 -1.334 -0.476 -0.445 0.5764 -0.5038 0.6434

72 H(1) Bbb -0.0003 -0.178 -0.063 -0.059 0.4181 0.8583 0.2975

Bcc 0.0028 1.511 0.539 0.504 -0.7021 0.0975 0.7054

Baa -0.0007 -0.365 -0.130 -0.122 -0.6037 0.7189 -0.3444

73 H(1) Bbb -0.0001 -0.067 -0.024 -0.022 -0.0466 0.3995 0.9156

Bcc 0.0008 0.432 0.154 0.144 0.7958 0.5688 -0.2077

Baa -0.0014 -0.739 -0.264 -0.246 -0.2905 0.3050 0.9070

74 H(1) Bbb -0.0004 -0.218 -0.078 -0.073 -0.6322 0.6503 -0.4212

Bcc 0.0018 0.957 0.341 0.319 0.7183 0.6958 -0.0039

Baa -0.0007 -0.360 -0.128 -0.120 0.6887 -0.6480 0.3254

75 H(1) Bbb -0.0002 -0.087 -0.031 -0.029 -0.3676 0.0748 0.9270

Bcc 0.0008 0.447 0.160 0.149 0.6250 0.7580 0.1867

Baa -0.0024 -1.276 -0.455 -0.426 -0.4482 0.6327 -0.6315

76 H(1) Bbb -0.0003 -0.182 -0.065 -0.061 0.8938 0.3267 -0.3071

Bcc 0.0027 1.458 0.520 0.486 -0.0120 0.7021 0.7120

Baa -0.0061 -3.247 -1.159 -1.083 -0.0000 -0.1019 0.9948

77 H(1) Bbb -0.0017 -0.889 -0.317 -0.296 1.0000 0.0000 0.0000

Bcc 0.0078 4.136 1.476 1.380 -0.0000 0.9948 0.1019

Baa -0.0061 -3.247 -1.159 -1.083 -0.0000 0.1019 0.9948

78 H(1) Bbb -0.0017 -0.889 -0.317 -0.296 1.0000 -0.0000 0.0000

Bcc 0.0078 4.136 1.476 1.380 0.0000 0.9948 -0.1019

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

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Sun Aug 18 13:47:46 2019, MaxMem= 2013265920 cpu: 36.3

(Enter /home/kira/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

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

GePol: Maximum number of non-zero 1st derivatives = 180

Leave Link 701 at Sun Aug 18 13:48:04 2019, MaxMem= 2013265920 cpu: 139.5

(Enter /home/kira/g09/l702.exe)

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

Leave Link 702 at Sun Aug 18 13:48:04 2019, MaxMem= 2013265920 cpu: 0.2

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

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

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

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Sun Aug 18 13:48:41 2019, MaxMem= 2013265920 cpu: 294.0

(Enter /home/kira/g09/l716.exe)

Dipole =-9.29287444D-13-1.23101529D-12-1.01347299D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.004603787 -0.002133445 -0.000254649

2 6 0.014962364 0.005220202 0.000134954

3 7 -0.000000000 0.001698529 -0.000352764

4 6 -0.014962364 0.005220202 0.000134954

5 6 0.004603787 -0.002133445 -0.000254649

6 6 0.006697245 -0.000427337 0.000054133

7 6 0.005238744 -0.003895070 -0.000053334

8 7 -0.002115999 -0.000000000 0.000974246

9 6 0.005238744 0.003895070 -0.000053334

10 6 -0.000639563 -0.000114044 0.000147018

11 6 -0.000639563 0.000114044 0.000147018

12 6 -0.006697245 -0.000427337 0.000054133

13 6 -0.005238744 -0.003895070 -0.000053334

14 6 0.000639563 0.000114044 0.000147018

15 6 0.000639563 -0.000114044 0.000147018

16 6 -0.005238744 0.003895070 -0.000053334

17 7 0.002115999 -0.000000000 0.000974246

18 6 -0.006697245 0.000427337 0.000054133

19 6 0.014962364 -0.005220202 0.000134954

20 6 -0.004603787 0.002133445 -0.000254649

21 6 0.004603787 0.002133445 -0.000254649

22 6 -0.014962364 -0.005220202 0.000134954

23 7 0.000000000 -0.001698529 -0.000352764

24 6 0.006697245 0.000427337 0.000054133

25 6 -0.000084422 -0.000168933 -0.000142408

26 6 -0.002024368 0.000876689 -0.001347178

27 6 -0.000092440 -0.000784643 -0.000042582

28 6 -0.000377621 -0.000332836 -0.000073076

29 6 -0.000872269 -0.000179515 0.000072812

30 6 0.000809805 -0.002058430 0.001330477

31 6 0.000377621 -0.000332836 -0.000073076

32 6 0.000092440 -0.000784643 -0.000042582

33 6 0.002024368 0.000876689 -0.001347178

34 6 0.000084422 -0.000168933 -0.000142408

35 6 -0.000809805 -0.002058430 0.001330477

36 6 0.000872269 -0.000179515 0.000072812

37 6 -0.000084422 0.000168933 -0.000142408

38 6 0.000809805 0.002058430 0.001330477

39 6 -0.000872269 0.000179515 0.000072812

40 6 -0.000377621 0.000332836 -0.000073076

41 6 -0.000092440 0.000784643 -0.000042582

42 6 -0.002024368 -0.000876689 -0.001347178

43 6 0.000084422 0.000168933 -0.000142408

44 6 -0.000809805 0.002058430 0.001330477

45 6 0.000872269 0.000179515 0.000072812

46 6 0.000377621 0.000332836 -0.000073076

47 6 0.000092440 0.000784643 -0.000042582

48 6 0.002024368 -0.000876689 -0.001347178

49 1 0.000223683 -0.000149638 0.000093630

50 1 -0.000223683 -0.000149638 0.000093630

51 1 -0.000339477 0.000214603 -0.000017651

52 1 -0.000339477 -0.000214603 -0.000017651

53 1 0.000339477 -0.000214603 -0.000017651

54 1 0.000339477 0.000214603 -0.000017651

55 1 0.000223683 0.000149638 0.000093630

56 1 -0.000223683 0.000149638 0.000093630

57 1 0.000097564 0.000137016 0.000030596

58 1 -0.000171175 -0.000358129 0.000086148

59 1 -0.000131660 -0.000134446 -0.000004897

60 1 -0.000369522 -0.000158730 -0.000082739

61 1 0.000140114 0.000087932 -0.000038540

62 1 0.000131660 -0.000134446 -0.000004897

63 1 0.000171175 -0.000358129 0.000086148

64 1 -0.000097564 0.000137016 0.000030596

65 1 -0.000140114 0.000087932 -0.000038540

66 1 0.000369522 -0.000158730 -0.000082739

67 1 0.000140114 -0.000087932 -0.000038540

68 1 -0.000369522 0.000158730 -0.000082739

69 1 -0.000131660 0.000134446 -0.000004897

70 1 -0.000171175 0.000358129 0.000086148

71 1 0.000097564 -0.000137016 0.000030596

72 1 -0.000140114 -0.000087932 -0.000038540

73 1 0.000369522 0.000158730 -0.000082739

74 1 0.000131660 0.000134446 -0.000004897

75 1 0.000171175 0.000358129 0.000086148

76 1 -0.000097564 -0.000137016 0.000030596

77 1 -0.000000000 -0.001119846 -0.000406911

78 1 -0.000000000 0.001119846 -0.000406911

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

Cartesian Forces: Max 0.014962364 RMS 0.002567832

Leave Link 716 at Sun Aug 18 13:48:41 2019, MaxMem= 2013265920 cpu: 0.2

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

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

Internal Forces: Max 0.007475017 RMS 0.001282216

Search for a local minimum.

Step number 1 out of a maximum of 452

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

RMS Force = .12822D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Second derivative matrix not updated -- first step.

ITU= 0

Eigenvalues --- 0.00861 0.00861 0.00861 0.00861 0.01643

Eigenvalues --- 0.01658 0.01665 0.01668 0.01686 0.01686

Eigenvalues --- 0.01708 0.01708 0.01708 0.01708 0.01716

Eigenvalues --- 0.01732 0.01802 0.01828 0.01829 0.01857

Eigenvalues --- 0.01870 0.01892 0.01907 0.01908 0.01943

Eigenvalues --- 0.01945 0.01994 0.01998 0.02008 0.02008

Eigenvalues --- 0.02021 0.02026 0.02041 0.02050 0.02062

Eigenvalues --- 0.02071 0.02075 0.02081 0.02096 0.02099

Eigenvalues --- 0.02099 0.02099 0.02099 0.02131 0.02131

Eigenvalues --- 0.02131 0.02131 0.02140 0.02140 0.02140

Eigenvalues --- 0.02140 0.02160 0.02160 0.02160 0.02160

Eigenvalues --- 0.02165 0.02165 0.02165 0.02165 0.02170

Eigenvalues --- 0.02170 0.02170 0.02170 0.02175 0.02175

Eigenvalues --- 0.02175 0.02175 0.02176 0.02176 0.02176

Eigenvalues --- 0.02176 0.02213 0.02213 0.02225 0.02225

Eigenvalues --- 0.15990 0.15990 0.15992 0.15992 0.15996

Eigenvalues --- 0.15996 0.15997 0.15997 0.15998 0.15998

Eigenvalues --- 0.15999 0.15999 0.15999 0.15999 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 0.16000 0.16000

Eigenvalues --- 0.22000 0.22000 0.22000 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22000 0.22774 0.22789

Eigenvalues --- 0.22797 0.22811 0.23475 0.23475 0.23475

Eigenvalues --- 0.23475 0.23540 0.23548 0.24743 0.24748

Eigenvalues --- 0.24862 0.24923 0.24958 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.33146 0.33146 0.33146

Eigenvalues --- 0.33146 0.34592 0.34622 0.35400 0.35400

Eigenvalues --- 0.35400 0.35400 0.35400 0.35400 0.35400

Eigenvalues --- 0.35400 0.35405 0.35405 0.35405 0.35405

Eigenvalues --- 0.35452 0.35452 0.35452 0.35452 0.35461

Eigenvalues --- 0.35461 0.35461 0.35461 0.36108 0.36108

Eigenvalues --- 0.36108 0.36108 0.36232 0.36232 0.36232

Eigenvalues --- 0.36232 0.36872 0.36882 0.37418 0.37449

Eigenvalues --- 0.39507 0.39662 0.42018 0.42018 0.42018

Eigenvalues --- 0.42018 0.42134 0.42134 0.42134 0.42134

Eigenvalues --- 0.43295 0.43531 0.44321 0.44398 0.44402

Eigenvalues --- 0.44419 0.45377 0.45481 0.45563 0.45566

Eigenvalues --- 0.45632 0.45632 0.45857 0.45857 0.45857

Eigenvalues --- 0.45857 0.46150 0.46150 0.46150 0.46150

Eigenvalues --- 0.46291 0.46645 0.46645 0.46645 0.46645

Eigenvalues --- 0.46835 0.46835 0.46835 0.46835 0.46922

Eigenvalues --- 0.48601 0.48655 0.49779 0.49884 0.50665

Eigenvalues --- 0.50731 0.53101 0.53112

RFO step: Lambda=-3.04689590D-03 EMin= 8.61370080D-03

Linear search not attempted -- first point.

Iteration 1 RMS(Cart)= 0.06226954 RMS(Int)= 0.00121562

Iteration 2 RMS(Cart)= 0.00211390 RMS(Int)= 0.00001174

Iteration 3 RMS(Cart)= 0.00000243 RMS(Int)= 0.00001169

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001169

ITry= 1 IFail=0 DXMaxC= 2.20D-01 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 9.78D-09 for atom 62.

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

(Linear) (Quad) (Total)

R1 2.70807 -0.00325 0.00000 -0.00768 -0.00768 2.70038

R2 2.58574 0.00092 0.00000 0.00249 0.00250 2.58823

R3 2.03720 -0.00025 0.00000 -0.00067 -0.00067 2.03653

R4 2.60062 -0.00400 0.00000 -0.00857 -0.00857 2.59205

R5 2.64624 0.00748 0.00000 0.01630 0.01630 2.66254

R6 2.60062 -0.00400 0.00000 -0.00857 -0.00857 2.59205

R7 1.91248 0.00114 0.00000 0.00249 0.00249 1.91497

R8 2.70807 -0.00325 0.00000 -0.00768 -0.00768 2.70038

R9 2.64624 0.00748 0.00000 0.01630 0.01630 2.66254

R10 2.03720 -0.00025 0.00000 -0.00067 -0.00067 2.03653

R11 2.65977 0.00063 0.00000 0.00141 0.00141 2.66118

R12 2.82096 -0.00435 0.00000 -0.01300 -0.01300 2.80795

R13 2.58380 -0.00195 0.00000 -0.00404 -0.00404 2.57976

R14 2.75572 -0.00120 0.00000 -0.00307 -0.00307 2.75265

R15 2.58380 -0.00195 0.00000 -0.00404 -0.00404 2.57976

R16 2.75572 -0.00120 0.00000 -0.00307 -0.00307 2.75265

R17 2.65977 0.00063 0.00000 0.00141 0.00141 2.66118

R18 2.56022 -0.00100 0.00000 -0.00151 -0.00150 2.55872

R19 2.03912 -0.00040 0.00000 -0.00109 -0.00109 2.03804

R20 2.03912 -0.00040 0.00000 -0.00109 -0.00109 2.03804

R21 2.65977 0.00063 0.00000 0.00141 0.00141 2.66118

R22 2.82096 -0.00435 0.00000 -0.01300 -0.01300 2.80795

R23 2.75572 -0.00120 0.00000 -0.00307 -0.00307 2.75265

R24 2.58380 -0.00195 0.00000 -0.00404 -0.00404 2.57976

R25 2.56022 -0.00100 0.00000 -0.00151 -0.00150 2.55872

R26 2.03912 -0.00040 0.00000 -0.00109 -0.00109 2.03804

R27 2.75572 -0.00120 0.00000 -0.00307 -0.00307 2.75265

R28 2.03912 -0.00040 0.00000 -0.00109 -0.00109 2.03804

R29 2.58380 -0.00195 0.00000 -0.00404 -0.00404 2.57976

R30 2.65977 0.00063 0.00000 0.00141 0.00141 2.66118

R31 2.64624 0.00748 0.00000 0.01630 0.01630 2.66254

R32 2.82096 -0.00435 0.00000 -0.01300 -0.01300 2.80795

R33 2.70807 -0.00325 0.00000 -0.00768 -0.00768 2.70038

R34 2.60062 -0.00400 0.00000 -0.00857 -0.00857 2.59205

R35 2.58574 0.00092 0.00000 0.00249 0.00250 2.58823

R36 2.03720 -0.00025 0.00000 -0.00067 -0.00067 2.03653

R37 2.70807 -0.00325 0.00000 -0.00768 -0.00768 2.70038

R38 2.03720 -0.00025 0.00000 -0.00067 -0.00067 2.03653

R39 2.60062 -0.00400 0.00000 -0.00857 -0.00857 2.59205

R40 2.64624 0.00748 0.00000 0.01630 0.01630 2.66254

R41 1.91248 0.00114 0.00000 0.00249 0.00249 1.91497

R42 2.82096 -0.00435 0.00000 -0.01300 -0.01300 2.80795

R43 2.64551 0.00001 0.00000 0.00009 0.00010 2.64561

R44 2.64582 -0.00007 0.00000 -0.00009 -0.00009 2.64573

R45 2.63223 -0.00137 0.00000 -0.00290 -0.00290 2.62934

R46 2.04948 -0.00009 0.00000 -0.00026 -0.00026 2.04921

R47 2.63457 0.00030 0.00000 0.00058 0.00057 2.63515

R48 2.05030 -0.00031 0.00000 -0.00086 -0.00086 2.04944

R49 2.63480 0.00040 0.00000 0.00078 0.00078 2.63558

R50 2.05022 -0.00019 0.00000 -0.00053 -0.00053 2.04969

R51 2.63180 -0.00143 0.00000 -0.00305 -0.00304 2.62875

R52 2.05030 -0.00031 0.00000 -0.00086 -0.00086 2.04944

R53 2.04933 -0.00010 0.00000 -0.00027 -0.00027 2.04906

R54 2.63457 0.00030 0.00000 0.00058 0.00057 2.63515

R55 2.63480 0.00040 0.00000 0.00078 0.00078 2.63558

R56 2.05022 -0.00019 0.00000 -0.00053 -0.00053 2.04969

R57 2.63223 -0.00137 0.00000 -0.00290 -0.00290 2.62934

R58 2.05030 -0.00031 0.00000 -0.00086 -0.00086 2.04944

R59 2.64551 0.00001 0.00000 0.00009 0.00010 2.64561

R60 2.04948 -0.00009 0.00000 -0.00026 -0.00026 2.04921

R61 2.64582 -0.00007 0.00000 -0.00009 -0.00009 2.64573

R62 2.63180 -0.00143 0.00000 -0.00305 -0.00304 2.62875

R63 2.04933 -0.00010 0.00000 -0.00027 -0.00027 2.04906

R64 2.05030 -0.00031 0.00000 -0.00086 -0.00086 2.04944

R65 2.64582 -0.00007 0.00000 -0.00009 -0.00009 2.64573

R66 2.64551 0.00001 0.00000 0.00009 0.00010 2.64561

R67 2.63180 -0.00143 0.00000 -0.00305 -0.00304 2.62875

R68 2.04933 -0.00010 0.00000 -0.00027 -0.00027 2.04906

R69 2.63480 0.00040 0.00000 0.00078 0.00078 2.63558

R70 2.05030 -0.00031 0.00000 -0.00086 -0.00086 2.04944

R71 2.63457 0.00030 0.00000 0.00058 0.00057 2.63515

R72 2.05022 -0.00019 0.00000 -0.00053 -0.00053 2.04969

R73 2.63223 -0.00137 0.00000 -0.00290 -0.00290 2.62934

R74 2.05030 -0.00031 0.00000 -0.00086 -0.00086 2.04944

R75 2.04948 -0.00009 0.00000 -0.00026 -0.00026 2.04921

R76 2.64582 -0.00007 0.00000 -0.00009 -0.00009 2.64573

R77 2.64551 0.00001 0.00000 0.00009 0.00010 2.64561

R78 2.63180 -0.00143 0.00000 -0.00305 -0.00304 2.62875

R79 2.04933 -0.00010 0.00000 -0.00027 -0.00027 2.04906

R80 2.63480 0.00040 0.00000 0.00078 0.00078 2.63558

R81 2.05030 -0.00031 0.00000 -0.00086 -0.00086 2.04944

R82 2.63457 0.00030 0.00000 0.00058 0.00057 2.63515

R83 2.05022 -0.00019 0.00000 -0.00053 -0.00053 2.04969

R84 2.63223 -0.00137 0.00000 -0.00290 -0.00290 2.62934

R85 2.05030 -0.00031 0.00000 -0.00086 -0.00086 2.04944

R86 2.04948 -0.00009 0.00000 -0.00026 -0.00026 2.04921

A1 1.88843 -0.00163 0.00000 -0.00518 -0.00519 1.88324

A2 2.17818 0.00091 0.00000 0.00316 0.00316 2.18134

A3 2.21648 0.00072 0.00000 0.00198 0.00198 2.21846

A4 1.85833 0.00262 0.00000 0.01023 0.01023 1.86857

A5 2.21343 -0.00180 0.00000 -0.00635 -0.00633 2.20710

A6 2.21142 -0.00082 0.00000 -0.00387 -0.00389 2.20752

A7 1.93111 -0.00197 0.00000 -0.01004 -0.01003 1.92108

A8 2.17584 0.00099 0.00000 0.00506 0.00506 2.18089

A9 2.17584 0.00099 0.00000 0.00506 0.00506 2.18089

A10 1.85833 0.00262 0.00000 0.01023 0.01023 1.86857

A11 2.21142 -0.00082 0.00000 -0.00387 -0.00389 2.20752

A12 2.21343 -0.00180 0.00000 -0.00635 -0.00633 2.20710

A13 1.88843 -0.00163 0.00000 -0.00518 -0.00519 1.88324

A14 2.21648 0.00072 0.00000 0.00198 0.00198 2.21846

A15 2.17818 0.00091 0.00000 0.00316 0.00316 2.18134

A16 2.18435 0.00223 0.00000 0.00786 0.00783 2.19219

A17 2.03707 -0.00108 0.00000 -0.00380 -0.00379 2.03328

A18 2.06176 -0.00115 0.00000 -0.00406 -0.00404 2.05771

A19 2.20254 -0.00345 0.00000 -0.01433 -0.01435 2.18819

A20 2.15052 0.00157 0.00000 0.00693 0.00695 2.15747

A21 1.93010 0.00189 0.00000 0.00742 0.00742 1.93752

A22 1.84760 -0.00203 0.00000 -0.00849 -0.00849 1.83912

A23 1.93010 0.00189 0.00000 0.00742 0.00742 1.93752

A24 2.20254 -0.00345 0.00000 -0.01433 -0.01435 2.18819

A25 2.15052 0.00157 0.00000 0.00693 0.00695 2.15747

A26 1.85833 -0.00087 0.00000 -0.00311 -0.00311 1.85522

A27 2.19869 0.00040 0.00000 0.00132 0.00132 2.20001

A28 2.22595 0.00047 0.00000 0.00175 0.00175 2.22770

A29 1.85833 -0.00087 0.00000 -0.00311 -0.00311 1.85522

A30 2.19869 0.00040 0.00000 0.00132 0.00132 2.20001

A31 2.22595 0.00047 0.00000 0.00175 0.00175 2.22770

A32 2.18435 0.00223 0.00000 0.00786 0.00783 2.19219

A33 2.03707 -0.00108 0.00000 -0.00380 -0.00379 2.03328

A34 2.06176 -0.00115 0.00000 -0.00406 -0.00404 2.05771

A35 2.15052 0.00157 0.00000 0.00693 0.00695 2.15747

A36 2.20254 -0.00345 0.00000 -0.01433 -0.01435 2.18819

A37 1.93010 0.00189 0.00000 0.00742 0.00742 1.93752

A38 1.85833 -0.00087 0.00000 -0.00311 -0.00311 1.85522

A39 2.19869 0.00040 0.00000 0.00132 0.00132 2.20001

A40 2.22595 0.00047 0.00000 0.00175 0.00175 2.22770

A41 1.85833 -0.00087 0.00000 -0.00311 -0.00311 1.85522

A42 2.22595 0.00047 0.00000 0.00175 0.00175 2.22770

A43 2.19869 0.00040 0.00000 0.00132 0.00132 2.20001

A44 1.93010 0.00189 0.00000 0.00742 0.00742 1.93752

A45 2.15052 0.00157 0.00000 0.00693 0.00695 2.15747

A46 2.20254 -0.00345 0.00000 -0.01433 -0.01435 2.18819

A47 1.84760 -0.00203 0.00000 -0.00849 -0.00849 1.83912

A48 2.18435 0.00223 0.00000 0.00786 0.00783 2.19219

A49 2.06176 -0.00115 0.00000 -0.00406 -0.00404 2.05771

A50 2.03707 -0.00108 0.00000 -0.00380 -0.00379 2.03328

A51 2.21343 -0.00180 0.00000 -0.00635 -0.00633 2.20710

A52 2.21142 -0.00082 0.00000 -0.00387 -0.00389 2.20752

A53 1.85833 0.00262 0.00000 0.01023 0.01023 1.86857

A54 1.88843 -0.00163 0.00000 -0.00518 -0.00519 1.88324

A55 2.17818 0.00091 0.00000 0.00316 0.00316 2.18134

A56 2.21648 0.00072 0.00000 0.00198 0.00198 2.21846

A57 1.88843 -0.00163 0.00000 -0.00518 -0.00519 1.88324

A58 2.21648 0.00072 0.00000 0.00198 0.00198 2.21846

A59 2.17818 0.00091 0.00000 0.00316 0.00316 2.18134

A60 1.85833 0.00262 0.00000 0.01023 0.01023 1.86857

A61 2.21343 -0.00180 0.00000 -0.00635 -0.00633 2.20710

A62 2.21142 -0.00082 0.00000 -0.00387 -0.00389 2.20752

A63 1.93111 -0.00197 0.00000 -0.01004 -0.01003 1.92108

A64 2.17584 0.00099 0.00000 0.00506 0.00506 2.18089

A65 2.17584 0.00099 0.00000 0.00506 0.00506 2.18089

A66 2.18435 0.00223 0.00000 0.00786 0.00783 2.19219

A67 2.06176 -0.00115 0.00000 -0.00406 -0.00404 2.05771

A68 2.03707 -0.00108 0.00000 -0.00380 -0.00379 2.03328

A69 2.10690 -0.00120 0.00000 -0.00496 -0.00496 2.10194

A70 2.10194 -0.00135 0.00000 -0.00555 -0.00555 2.09639

A71 2.07434 0.00255 0.00000 0.01051 0.01051 2.08485

A72 2.10442 -0.00160 0.00000 -0.00681 -0.00682 2.09760

A73 2.08445 0.00094 0.00000 0.00424 0.00423 2.08869

A74 2.09426 0.00066 0.00000 0.00251 0.00251 2.09677

A75 2.09712 -0.00009 0.00000 -0.00030 -0.00032 2.09680

A76 2.08912 -0.00021 0.00000 -0.00144 -0.00143 2.08769

A77 2.09694 0.00031 0.00000 0.00175 0.00175 2.09870

A78 2.08887 0.00081 0.00000 0.00358 0.00357 2.09243

A79 2.09716 -0.00040 0.00000 -0.00180 -0.00179 2.09537

A80 2.09715 -0.00040 0.00000 -0.00178 -0.00178 2.09538

A81 2.09703 -0.00006 0.00000 -0.00018 -0.00020 2.09683

A82 2.09694 0.00029 0.00000 0.00171 0.00172 2.09866

A83 2.08922 -0.00023 0.00000 -0.00153 -0.00152 2.08769

A84 2.10459 -0.00161 0.00000 -0.00687 -0.00688 2.09771

A85 2.08384 0.00094 0.00000 0.00423 0.00422 2.08806

A86 2.09473 0.00067 0.00000 0.00260 0.00259 2.09733

A87 2.08887 0.00081 0.00000 0.00358 0.00357 2.09243

A88 2.09716 -0.00040 0.00000 -0.00180 -0.00179 2.09537

A89 2.09715 -0.00040 0.00000 -0.00178 -0.00178 2.09538

A90 2.09712 -0.00009 0.00000 -0.00030 -0.00032 2.09680

A91 2.09694 0.00031 0.00000 0.00175 0.00175 2.09870

A92 2.08912 -0.00021 0.00000 -0.00144 -0.00143 2.08769

A93 2.10442 -0.00160 0.00000 -0.00681 -0.00682 2.09760

A94 2.09426 0.00066 0.00000 0.00251 0.00251 2.09677

A95 2.08445 0.00094 0.00000 0.00424 0.00423 2.08869

A96 2.10690 -0.00120 0.00000 -0.00496 -0.00496 2.10194

A97 2.10194 -0.00135 0.00000 -0.00555 -0.00555 2.09639

A98 2.07434 0.00255 0.00000 0.01051 0.01051 2.08485

A99 2.10459 -0.00161 0.00000 -0.00687 -0.00688 2.09771

A100 2.08384 0.00094 0.00000 0.00423 0.00422 2.08806

A101 2.09473 0.00067 0.00000 0.00260 0.00259 2.09733

A102 2.09703 -0.00006 0.00000 -0.00018 -0.00020 2.09683

A103 2.09694 0.00029 0.00000 0.00171 0.00172 2.09866

A104 2.08922 -0.00023 0.00000 -0.00153 -0.00152 2.08769

A105 2.10194 -0.00135 0.00000 -0.00555 -0.00555 2.09639

A106 2.10690 -0.00120 0.00000 -0.00496 -0.00496 2.10194

A107 2.07434 0.00255 0.00000 0.01051 0.01051 2.08485

A108 2.10459 -0.00161 0.00000 -0.00687 -0.00688 2.09771

A109 2.08384 0.00094 0.00000 0.00423 0.00422 2.08806

A110 2.09473 0.00067 0.00000 0.00260 0.00259 2.09733

A111 2.09703 -0.00006 0.00000 -0.00018 -0.00020 2.09683

A112 2.08922 -0.00023 0.00000 -0.00153 -0.00152 2.08769

A113 2.09694 0.00029 0.00000 0.00171 0.00172 2.09866

A114 2.08887 0.00081 0.00000 0.00358 0.00357 2.09243

A115 2.09715 -0.00040 0.00000 -0.00178 -0.00178 2.09538

A116 2.09716 -0.00040 0.00000 -0.00180 -0.00179 2.09537

A117 2.09712 -0.00009 0.00000 -0.00030 -0.00032 2.09680

A118 2.09694 0.00031 0.00000 0.00175 0.00175 2.09870

A119 2.08912 -0.00021 0.00000 -0.00144 -0.00143 2.08769

A120 2.10442 -0.00160 0.00000 -0.00681 -0.00682 2.09760

A121 2.08445 0.00094 0.00000 0.00424 0.00423 2.08869

A122 2.09426 0.00066 0.00000 0.00251 0.00251 2.09677

A123 2.10194 -0.00135 0.00000 -0.00555 -0.00555 2.09639

A124 2.10690 -0.00120 0.00000 -0.00496 -0.00496 2.10194

A125 2.07434 0.00255 0.00000 0.01051 0.01051 2.08485

A126 2.10459 -0.00161 0.00000 -0.00687 -0.00688 2.09771

A127 2.08384 0.00094 0.00000 0.00423 0.00422 2.08806

A128 2.09473 0.00067 0.00000 0.00260 0.00259 2.09733

A129 2.09703 -0.00006 0.00000 -0.00018 -0.00020 2.09683

A130 2.08922 -0.00023 0.00000 -0.00153 -0.00152 2.08769

A131 2.09694 0.00029 0.00000 0.00171 0.00172 2.09866

A132 2.08887 0.00081 0.00000 0.00358 0.00357 2.09243

A133 2.09715 -0.00040 0.00000 -0.00178 -0.00178 2.09538

A134 2.09716 -0.00040 0.00000 -0.00180 -0.00179 2.09537

A135 2.09712 -0.00009 0.00000 -0.00030 -0.00032 2.09680

A136 2.09694 0.00031 0.00000 0.00175 0.00175 2.09870

A137 2.08912 -0.00021 0.00000 -0.00144 -0.00143 2.08769

A138 2.10442 -0.00160 0.00000 -0.00681 -0.00682 2.09760

A139 2.08445 0.00094 0.00000 0.00424 0.00423 2.08869

A140 2.09426 0.00066 0.00000 0.00251 0.00251 2.09677

D1 0.00925 -0.00005 0.00000 -0.00238 -0.00240 0.00685

D2 -3.13580 0.00004 0.00000 0.00138 0.00137 -3.13443

D3 -3.11864 0.00002 0.00000 0.00067 0.00067 -3.11797

D4 0.01950 0.00011 0.00000 0.00443 0.00443 0.02393

D5 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D6 -3.12750 0.00007 0.00000 0.00313 0.00314 -3.12436

D7 3.12750 -0.00007 0.00000 -0.00313 -0.00314 3.12436

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 -0.01544 0.00009 0.00000 0.00407 0.00407 -0.01137

D10 3.09677 0.00017 0.00000 0.00743 0.00744 3.10421

D11 3.12961 0.00001 0.00000 0.00032 0.00031 3.12991

D12 -0.04137 0.00009 0.00000 0.00369 0.00368 -0.03769

D13 -3.07513 0.00030 0.00000 0.01226 0.01227 -3.06286

D14 0.06262 0.00030 0.00000 0.01244 0.01245 0.07507

D15 0.06233 0.00041 0.00000 0.01678 0.01677 0.07910

D16 -3.08310 0.00041 0.00000 0.01696 0.01695 -3.06615

D17 0.01544 -0.00009 0.00000 -0.00407 -0.00407 0.01137

D18 -3.12961 -0.00001 0.00000 -0.00032 -0.00031 -3.12991

D19 -3.09677 -0.00017 0.00000 -0.00743 -0.00744 -3.10421

D20 0.04137 -0.00009 0.00000 -0.00369 -0.00368 0.03769

D21 -0.00925 0.00005 0.00000 0.00238 0.00240 -0.00685

D22 3.11864 -0.00002 0.00000 -0.00067 -0.00067 3.11797

D23 3.13580 -0.00004 0.00000 -0.00138 -0.00137 3.13443

D24 -0.01950 -0.00011 0.00000 -0.00443 -0.00443 -0.02393

D25 -0.06233 -0.00041 0.00000 -0.01678 -0.01677 -0.07910

D26 3.08310 -0.00041 0.00000 -0.01696 -0.01695 3.06615

D27 3.07513 -0.00030 0.00000 -0.01226 -0.01227 3.06286

D28 -0.06262 -0.00030 0.00000 -0.01244 -0.01245 -0.07507

D29 -0.08048 -0.00025 0.00000 -0.01097 -0.01095 -0.09143

D30 3.05406 -0.00012 0.00000 -0.00520 -0.00521 3.04885

D31 3.05723 -0.00025 0.00000 -0.01078 -0.01077 3.04646

D32 -0.09142 -0.00012 0.00000 -0.00501 -0.00502 -0.09644

D33 -1.13207 0.00075 0.00000 0.06400 0.06400 -1.06807

D34 2.00962 0.00074 0.00000 0.06331 0.06331 2.07293

D35 2.01309 0.00074 0.00000 0.06380 0.06380 2.07689

D36 -1.12841 0.00073 0.00000 0.06312 0.06312 -1.06529

D37 -3.12515 0.00000 0.00000 0.00003 0.00001 -3.12515

D38 0.02275 -0.00012 0.00000 -0.00514 -0.00513 0.01762

D39 3.13338 -0.00004 0.00000 -0.00173 -0.00176 3.13161

D40 -0.02882 -0.00008 0.00000 -0.00379 -0.00382 -0.03264

D41 -0.01430 0.00006 0.00000 0.00316 0.00317 -0.01113

D42 3.10669 0.00002 0.00000 0.00110 0.00112 3.10781

D43 -0.02275 0.00012 0.00000 0.00514 0.00513 -0.01762

D44 3.12515 -0.00000 0.00000 -0.00003 -0.00001 3.12515

D45 0.01430 -0.00006 0.00000 -0.00316 -0.00317 0.01113

D46 -3.10669 -0.00002 0.00000 -0.00110 -0.00112 -3.10781

D47 -3.13338 0.00004 0.00000 0.00173 0.00176 -3.13161

D48 0.02882 0.00008 0.00000 0.00379 0.00382 0.03264

D49 0.08048 0.00025 0.00000 0.01097 0.01095 0.09143

D50 -3.05723 0.00025 0.00000 0.01078 0.01077 -3.04646

D51 -3.05406 0.00012 0.00000 0.00520 0.00521 -3.04885

D52 0.09142 0.00012 0.00000 0.00501 0.00502 0.09644

D53 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D54 -3.12056 0.00005 0.00000 0.00211 0.00210 -3.11846

D55 3.12056 -0.00005 0.00000 -0.00211 -0.00210 3.11846

D56 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D57 -3.05406 0.00012 0.00000 0.00520 0.00521 -3.04885

D58 0.08048 0.00025 0.00000 0.01097 0.01095 0.09143

D59 0.09142 0.00012 0.00000 0.00501 0.00502 0.09644

D60 -3.05723 0.00025 0.00000 0.01078 0.01077 -3.04646

D61 1.13207 -0.00075 0.00000 -0.06400 -0.06400 1.06807

D62 -2.00962 -0.00074 0.00000 -0.06331 -0.06331 -2.07293

D63 -2.01309 -0.00074 0.00000 -0.06380 -0.06380 -2.07689

D64 1.12841 -0.00073 0.00000 -0.06312 -0.06312 1.06529

D65 -3.13338 0.00004 0.00000 0.00173 0.00176 -3.13161

D66 0.02882 0.00008 0.00000 0.00379 0.00382 0.03264

D67 0.01430 -0.00006 0.00000 -0.00316 -0.00317 0.01113

D68 -3.10669 -0.00002 0.00000 -0.00110 -0.00112 -3.10781

D69 3.12515 -0.00000 0.00000 -0.00003 -0.00001 3.12515

D70 -0.02275 0.00012 0.00000 0.00514 0.00513 -0.01762

D71 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D72 -3.12056 0.00005 0.00000 0.00211 0.00210 -3.11846

D73 3.12056 -0.00005 0.00000 -0.00211 -0.00210 3.11846

D74 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D75 -0.01430 0.00006 0.00000 0.00316 0.00317 -0.01113

D76 3.13338 -0.00004 0.00000 -0.00173 -0.00176 3.13161

D77 3.10669 0.00002 0.00000 0.00110 0.00112 3.10781

D78 -0.02882 -0.00008 0.00000 -0.00379 -0.00382 -0.03264

D79 0.02275 -0.00012 0.00000 -0.00514 -0.00513 0.01762

D80 -3.12515 0.00000 0.00000 0.00003 0.00001 -3.12515

D81 3.05406 -0.00012 0.00000 -0.00520 -0.00521 3.04885

D82 -0.09142 -0.00012 0.00000 -0.00501 -0.00502 -0.09644

D83 -0.08048 -0.00025 0.00000 -0.01097 -0.01095 -0.09143

D84 3.05723 -0.00025 0.00000 -0.01078 -0.01077 3.04646

D85 3.07513 -0.00030 0.00000 -0.01226 -0.01227 3.06286

D86 -0.06233 -0.00041 0.00000 -0.01678 -0.01677 -0.07910

D87 -0.06262 -0.00030 0.00000 -0.01244 -0.01245 -0.07507

D88 3.08310 -0.00041 0.00000 -0.01696 -0.01695 3.06615

D89 -1.12841 0.00073 0.00000 0.06312 0.06312 -1.06529

D90 2.01309 0.00074 0.00000 0.06380 0.06380 2.07689

D91 2.00962 0.00074 0.00000 0.06331 0.06331 2.07293

D92 -1.13207 0.00075 0.00000 0.06400 0.06400 -1.06807

D93 3.13580 -0.00004 0.00000 -0.00138 -0.00137 3.13443

D94 -0.01950 -0.00011 0.00000 -0.00443 -0.00443 -0.02393

D95 -0.00925 0.00005 0.00000 0.00238 0.00240 -0.00685

D96 3.11864 -0.00002 0.00000 -0.00067 -0.00067 3.11797

D97 -3.12961 -0.00001 0.00000 -0.00032 -0.00031 -3.12991

D98 0.04137 -0.00009 0.00000 -0.00369 -0.00368 0.03769

D99 0.01544 -0.00009 0.00000 -0.00407 -0.00407 0.01137

D100 -3.09677 -0.00017 0.00000 -0.00743 -0.00744 -3.10421

D101 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D102 3.12750 -0.00007 0.00000 -0.00313 -0.00314 3.12436

D103 -3.12750 0.00007 0.00000 0.00313 0.00314 -3.12436

D104 -0.00000 0.00000 0.00000 0.00000 -0.00000 -0.00000

D105 0.00925 -0.00005 0.00000 -0.00238 -0.00240 0.00685

D106 -3.13580 0.00004 0.00000 0.00138 0.00137 -3.13443

D107 -3.11864 0.00002 0.00000 0.00067 0.00067 -3.11797

D108 0.01950 0.00011 0.00000 0.00443 0.00443 0.02393

D109 -0.01544 0.00009 0.00000 0.00407 0.00407 -0.01137

D110 3.09677 0.00017 0.00000 0.00743 0.00744 3.10421

D111 3.12961 0.00001 0.00000 0.00032 0.00031 3.12991

D112 -0.04137 0.00009 0.00000 0.00369 0.00368 -0.03769

D113 -3.07513 0.00030 0.00000 0.01226 0.01227 -3.06286

D114 0.06262 0.00030 0.00000 0.01244 0.01245 0.07507

D115 0.06233 0.00041 0.00000 0.01678 0.01677 0.07910

D116 -3.08310 0.00041 0.00000 0.01696 0.01695 -3.06615

D117 1.12841 -0.00073 0.00000 -0.06312 -0.06312 1.06529

D118 -2.01309 -0.00074 0.00000 -0.06380 -0.06380 -2.07689

D119 -2.00962 -0.00074 0.00000 -0.06331 -0.06331 -2.07293

D120 1.13207 -0.00075 0.00000 -0.06400 -0.06400 1.06807

D121 -3.13882 0.00013 0.00000 0.00505 0.00505 -3.13377

D122 -0.00768 -0.00003 0.00000 -0.00133 -0.00132 -0.00900

D123 0.00268 0.00014 0.00000 0.00573 0.00572 0.00841

D124 3.13382 -0.00002 0.00000 -0.00065 -0.00064 3.13317

D125 -3.14039 0.00015 0.00000 0.00634 0.00634 -3.13405

D126 -0.00650 -0.00001 0.00000 -0.00022 -0.00022 -0.00672

D127 0.00130 0.00014 0.00000 0.00566 0.00566 0.00696

D128 3.13519 -0.00002 0.00000 -0.00090 -0.00089 3.13429

D129 -0.00440 -0.00028 0.00000 -0.01134 -0.01132 -0.01573

D130 3.13434 -0.00014 0.00000 -0.00591 -0.00589 3.12845

D131 -3.13548 -0.00012 0.00000 -0.00494 -0.00493 -3.14041

D132 0.00327 0.00001 0.00000 0.00049 0.00050 0.00376

D133 0.00211 0.00014 0.00000 0.00552 0.00555 0.00765

D134 -3.13972 0.00014 0.00000 0.00564 0.00567 -3.13405

D135 -3.13663 0.00000 0.00000 0.00007 0.00009 -3.13654

D136 0.00474 0.00001 0.00000 0.00020 0.00021 0.00495

D137 0.00186 0.00015 0.00000 0.00584 0.00587 0.00773

D138 -3.13745 0.00001 0.00000 0.00055 0.00056 -3.13689

D139 -3.13950 0.00014 0.00000 0.00572 0.00575 -3.13375

D140 0.00437 0.00001 0.00000 0.00043 0.00044 0.00481

D141 -0.00358 -0.00028 0.00000 -0.01148 -0.01146 -0.01504

D142 -3.13742 -0.00012 0.00000 -0.00488 -0.00488 3.14089

D143 3.13575 -0.00015 0.00000 -0.00620 -0.00618 3.12957

D144 0.00191 0.00001 0.00000 0.00039 0.00040 0.00231

D145 -0.00211 -0.00014 0.00000 -0.00552 -0.00555 -0.00765

D146 3.13663 -0.00000 0.00000 -0.00007 -0.00009 3.13654

D147 3.13972 -0.00014 0.00000 -0.00564 -0.00567 3.13405

D148 -0.00474 -0.00001 0.00000 -0.00020 -0.00021 -0.00495

D149 -0.00186 -0.00015 0.00000 -0.00584 -0.00587 -0.00773

D150 3.13745 -0.00001 0.00000 -0.00055 -0.00056 3.13689

D151 3.13950 -0.00014 0.00000 -0.00572 -0.00575 3.13375

D152 -0.00437 -0.00001 0.00000 -0.00043 -0.00044 -0.00481

D153 0.00440 0.00028 0.00000 0.01134 0.01132 0.01573

D154 3.13548 0.00012 0.00000 0.00494 0.00493 3.14041

D155 -3.13434 0.00014 0.00000 0.00591 0.00589 -3.12845

D156 -0.00327 -0.00001 0.00000 -0.00049 -0.00050 -0.00376

D157 3.13882 -0.00013 0.00000 -0.00505 -0.00505 3.13377

D158 -0.00268 -0.00014 0.00000 -0.00573 -0.00572 -0.00841

D159 0.00768 0.00003 0.00000 0.00133 0.00132 0.00900

D160 -3.13382 0.00002 0.00000 0.00065 0.00064 -3.13317

D161 3.14039 -0.00015 0.00000 -0.00634 -0.00634 3.13405

D162 0.00650 0.00001 0.00000 0.00022 0.00022 0.00672

D163 -0.00130 -0.00014 0.00000 -0.00566 -0.00566 -0.00696

D164 -3.13519 0.00002 0.00000 0.00090 0.00089 -3.13429

D165 0.00358 0.00028 0.00000 0.01148 0.01146 0.01504

D166 -3.13575 0.00015 0.00000 0.00620 0.00618 -3.12957

D167 3.13742 0.00012 0.00000 0.00488 0.00488 -3.14089

D168 -0.00191 -0.00001 0.00000 -0.00039 -0.00040 -0.00231

D169 3.14039 -0.00015 0.00000 -0.00634 -0.00634 3.13405

D170 0.00650 0.00001 0.00000 0.00022 0.00022 0.00672

D171 -0.00130 -0.00014 0.00000 -0.00566 -0.00566 -0.00696

D172 -3.13519 0.00002 0.00000 0.00090 0.00089 -3.13429

D173 3.13882 -0.00013 0.00000 -0.00505 -0.00505 3.13377

D174 0.00768 0.00003 0.00000 0.00133 0.00132 0.00900

D175 -0.00268 -0.00014 0.00000 -0.00573 -0.00572 -0.00841

D176 -3.13382 0.00002 0.00000 0.00065 0.00064 -3.13317

D177 0.00358 0.00028 0.00000 0.01148 0.01146 0.01504

D178 -3.13575 0.00015 0.00000 0.00620 0.00618 -3.12957

D179 3.13742 0.00012 0.00000 0.00488 0.00488 -3.14089

D180 -0.00191 -0.00001 0.00000 -0.00039 -0.00040 -0.00231

D181 -0.00186 -0.00015 0.00000 -0.00584 -0.00587 -0.00773

D182 3.13950 -0.00014 0.00000 -0.00572 -0.00575 3.13375

D183 3.13745 -0.00001 0.00000 -0.00055 -0.00056 3.13689

D184 -0.00437 -0.00001 0.00000 -0.00043 -0.00044 -0.00481

D185 -0.00211 -0.00014 0.00000 -0.00552 -0.00555 -0.00765

D186 3.13663 -0.00000 0.00000 -0.00007 -0.00009 3.13654

D187 3.13972 -0.00014 0.00000 -0.00564 -0.00567 3.13405

D188 -0.00474 -0.00001 0.00000 -0.00020 -0.00021 -0.00495

D189 0.00440 0.00028 0.00000 0.01134 0.01132 0.01573

D190 3.13548 0.00012 0.00000 0.00494 0.00493 3.14041

D191 -3.13434 0.00014 0.00000 0.00591 0.00589 -3.12845

D192 -0.00327 -0.00001 0.00000 -0.00049 -0.00050 -0.00376

D193 -3.14039 0.00015 0.00000 0.00634 0.00634 -3.13405

D194 -0.00650 -0.00001 0.00000 -0.00022 -0.00022 -0.00672

D195 0.00130 0.00014 0.00000 0.00566 0.00566 0.00696

D196 3.13519 -0.00002 0.00000 -0.00090 -0.00089 3.13429

D197 -3.13882 0.00013 0.00000 0.00505 0.00505 -3.13377

D198 -0.00768 -0.00003 0.00000 -0.00133 -0.00132 -0.00900

D199 0.00268 0.00014 0.00000 0.00573 0.00572 0.00841

D200 3.13382 -0.00002 0.00000 -0.00065 -0.00064 3.13317

D201 -0.00358 -0.00028 0.00000 -0.01148 -0.01146 -0.01504

D202 3.13575 -0.00015 0.00000 -0.00620 -0.00618 3.12957

D203 -3.13742 -0.00012 0.00000 -0.00488 -0.00488 3.14089

D204 0.00191 0.00001 0.00000 0.00039 0.00040 0.00231

D205 0.00186 0.00015 0.00000 0.00584 0.00587 0.00773

D206 -3.13950 0.00014 0.00000 0.00572 0.00575 -3.13375

D207 -3.13745 0.00001 0.00000 0.00055 0.00056 -3.13689

D208 0.00437 0.00001 0.00000 0.00043 0.00044 0.00481

D209 0.00211 0.00014 0.00000 0.00552 0.00555 0.00765

D210 -3.13663 0.00000 0.00000 0.00007 0.00009 -3.13654

D211 -3.13972 0.00014 0.00000 0.00564 0.00567 -3.13405

D212 0.00474 0.00001 0.00000 0.00020 0.00021 0.00495

D213 -0.00440 -0.00028 0.00000 -0.01134 -0.01132 -0.01573

D214 -3.13548 -0.00012 0.00000 -0.00494 -0.00493 -3.14041

D215 3.13434 -0.00014 0.00000 -0.00591 -0.00589 3.12845

D216 0.00327 0.00001 0.00000 0.00049 0.00050 0.00376

Item Value Threshold Converged?

Maximum Force 0.007475 0.000450 NO

RMS Force 0.001282 0.000300 NO

Maximum Displacement 0.219773 0.001800 NO

RMS Displacement 0.062857 0.001200 NO

Predicted change in Energy=-1.644259D-03

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Aug 18 13:48:41 2019, MaxMem= 2013265920 cpu: 1.8

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

Stoichiometry C44H30N4(1+,2)

Framework group C2V[SGV(H2N2),SGV'(N2),X(C44H28)]

Deg. of freedom 59

Full point group C2V NOp 4

RotChk: IX=0 Diff= 3.20D-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 -0.684817 4.225596 0.204147

2 6 0 -1.124071 2.874627 0.049470

3 7 0 0.000000 2.092696 -0.031020

4 6 0 1.124071 2.874627 0.049470

5 6 0 0.684817 4.225596 0.204147

6 6 0 2.459754 2.430091 -0.009591

7 6 0 2.874341 1.085750 -0.072734

8 7 0 2.051479 -0.000000 0.014897

9 6 0 2.874341 -1.085750 -0.072734

10 6 0 4.261856 -0.677009 -0.244589

11 6 0 4.261856 0.677009 -0.244589

12 6 0 -2.459754 2.430091 -0.009591

13 6 0 -2.874341 1.085750 -0.072734

14 6 0 -4.261856 0.677009 -0.244589

15 6 0 -4.261856 -0.677009 -0.244589

16 6 0 -2.874341 -1.085750 -0.072734

17 7 0 -2.051479 0.000000 0.014897

18 6 0 -2.459754 -2.430091 -0.009591

19 6 0 -1.124071 -2.874627 0.049470

20 6 0 -0.684817 -4.225596 0.204147

21 6 0 0.684817 -4.225596 0.204147

22 6 0 1.124071 -2.874627 0.049470

23 7 0 -0.000000 -2.092696 -0.031020

24 6 0 2.459754 -2.430091 -0.009591

25 6 0 3.509531 3.481646 0.000898

26 6 0 3.566863 4.436642 -1.021200

27 6 0 4.557734 5.413384 -1.011200

28 6 0 5.487310 5.457069 0.027307

29 6 0 5.428446 4.513708 1.052861

30 6 0 4.450496 3.524544 1.036714

31 6 0 -5.487310 5.457069 0.027307

32 6 0 -4.557734 5.413384 -1.011200

33 6 0 -3.566863 4.436642 -1.021200

34 6 0 -3.509531 3.481646 0.000898

35 6 0 -4.450496 3.524544 1.036714

36 6 0 -5.428446 4.513708 1.052861

37 6 0 3.509531 -3.481646 0.000898

38 6 0 4.450496 -3.524544 1.036714

39 6 0 5.428446 -4.513708 1.052861

40 6 0 5.487310 -5.457069 0.027307

41 6 0 4.557734 -5.413384 -1.011200

42 6 0 3.566863 -4.436642 -1.021200

43 6 0 -3.509531 -3.481646 0.000898

44 6 0 -4.450496 -3.524544 1.036714

45 6 0 -5.428446 -4.513708 1.052861

46 6 0 -5.487310 -5.457069 0.027307

47 6 0 -4.557734 -5.413384 -1.011200

48 6 0 -3.566863 -4.436642 -1.021200

49 1 0 -1.335012 5.077652 0.316610

50 1 0 1.335012 5.077652 0.316610

51 1 0 5.106760 -1.335604 -0.369143

52 1 0 5.106760 1.335604 -0.369143

53 1 0 -5.106760 1.335604 -0.369143

54 1 0 -5.106760 -1.335604 -0.369143

55 1 0 -1.335012 -5.077652 0.316610

56 1 0 1.335012 -5.077652 0.316610

57 1 0 2.844661 4.402017 -1.829372

58 1 0 4.600991 6.141187 -1.814072

59 1 0 6.254897 6.223343 0.037440

60 1 0 6.145796 4.544943 1.865643

61 1 0 4.404710 2.790492 1.833465

62 1 0 -6.254897 6.223343 0.037440

63 1 0 -4.600991 6.141187 -1.814072

64 1 0 -2.844661 4.402017 -1.829372

65 1 0 -4.404710 2.790492 1.833465

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73 1 0 -6.145796 -4.544943 1.865643

74 1 0 -6.254897 -6.223343 0.037440

75 1 0 -4.600991 -6.141187 -1.814072

76 1 0 -2.844661 -4.402017 -1.829372

77 1 0 0.000000 1.082682 -0.113270

78 1 0 -0.000000 -1.082682 -0.113270

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

Rotational constants (GHZ): 0.0590786 0.0584091 0.0303029

Leave Link 202 at Sun Aug 18 13:48:41 2019, MaxMem= 2013265920 cpu: 0.1

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

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

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

There are 261 symmetry adapted cartesian basis functions of A1 symmetry.

There are 240 symmetry adapted cartesian basis functions of A2 symmetry.

There are 249 symmetry adapted cartesian basis functions of B1 symmetry.

There are 252 symmetry adapted cartesian basis functions of B2 symmetry.

There are 248 symmetry adapted basis functions of A1 symmetry.

There are 229 symmetry adapted basis functions of A2 symmetry.

There are 237 symmetry adapted basis functions of B1 symmetry.

There are 240 symmetry adapted basis functions of B2 symmetry.

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

161 alpha electrons 160 beta electrons

nuclear repulsion energy 5369.4211653978 Hartrees.

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

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

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

NAtoms= 78 NActive= 78 NUniq= 21 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=T Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2127781857 Hartrees.

Nuclear repulsion after empirical dispersion term = 5369.2083872122 Hartrees.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 78

GePol: Total number of spheres = 78

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

GePol: Number of points = 5738

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.25D-09

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 318

GePol: Fraction of low-weight points (<1% of avg) = 5.54%

GePol: Cavity surface area = 611.123 Ang\*\*2

GePol: Cavity volume = 625.294 Ang\*\*3

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

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

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PCM non-electrostatic energy = -0.0021528079 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5369.2062344043 Hartrees.

Leave Link 301 at Sun Aug 18 13:48:41 2019, MaxMem= 2013265920 cpu: 1.0

(Enter /home/kira/g09/l302.exe)

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

NBasis= 954 RedAO= T EigKep= 6.15D-05 NBF= 248 229 237 240

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 248 229 237 240

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= 941 941 941 941 941 MxSgAt= 78 MxSgA2= 78.

Leave Link 302 at Sun Aug 18 13:48:42 2019, MaxMem= 2013265920 cpu: 9.8

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

DipDrv: MaxL=1.

Leave Link 303 at Sun Aug 18 13:48:42 2019, MaxMem= 2013265920 cpu: 1.3

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

Initial guess from the checkpoint file: "TPPcation.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-A1.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7890 S= 0.5193

Generating alternative initial guess.

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -1914.09237152694

Leave Link 401 at Sun Aug 18 13:48:48 2019, MaxMem= 2013265920 cpu: 44.9

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3049894 IEndB= 3049894 NGot= 2013265920 MDV= 2011237673

LenX= 2011237673 LenY= 2010232667

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

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

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

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

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

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 98773932.

Iteration 1 A\*A^-1 deviation from unit magnitude is 1.03D-14 for 5716.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.22D-15 for 4896 3317.

Iteration 1 A^-1\*A deviation from unit magnitude is 1.09D-14 for 5716.

Iteration 1 A^-1\*A deviation from orthogonality is 1.12D-14 for 1922 1920.

E= -1914.16715822099

DIIS: error= 7.19D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.16715822099 IErMin= 1 ErrMin= 7.19D-03

ErrMax= 7.19D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.96D-02 BMatP= 5.96D-02

IDIUse=3 WtCom= 9.28D-01 WtEn= 7.19D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.506 Goal= None Shift= 0.000

Gap= 0.515 Goal= None Shift= 0.000

GapD= 0.506 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=1.87D-04 MaxDP=5.02D-03 OVMax= 3.34D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.87D-04 CP: 9.99D-01

E= -1914.19933037239 Delta-E= -0.032172151403 Rises=F Damp=F

DIIS: error= 9.45D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.19933037239 IErMin= 2 ErrMin= 9.45D-04

ErrMax= 9.45D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.09D-03 BMatP= 5.96D-02

IDIUse=3 WtCom= 9.91D-01 WtEn= 9.45D-03

Coeff-Com: -0.628D-01 0.106D+01

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

Coeff: -0.622D-01 0.106D+01

Gap= 0.101 Goal= None Shift= 0.000

Gap= 0.053 Goal= None Shift= 0.000

RMSDP=3.53D-05 MaxDP=1.49D-03 DE=-3.22D-02 OVMax= 5.25D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.33D-05 CP: 9.99D-01 1.06D+00

E= -1914.19981126778 Delta-E= -0.000480895394 Rises=F Damp=F

DIIS: error= 4.61D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.19981126778 IErMin= 3 ErrMin= 4.61D-04

ErrMax= 4.61D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.40D-04 BMatP= 1.09D-03

IDIUse=3 WtCom= 9.95D-01 WtEn= 4.61D-03

Coeff-Com: -0.386D-01 0.486D+00 0.553D+00

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

Coeff: -0.384D-01 0.484D+00 0.555D+00

Gap= 0.101 Goal= None Shift= 0.000

Gap= 0.054 Goal= None Shift= 0.000

RMSDP=1.32D-05 MaxDP=1.35D-03 DE=-4.81D-04 OVMax= 3.00D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.09D-05 CP: 9.99D-01 1.08D+00 7.89D-01

E= -1914.19993729287 Delta-E= -0.000126025091 Rises=F Damp=F

DIIS: error= 1.87D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.19993729287 IErMin= 4 ErrMin= 1.87D-04

ErrMax= 1.87D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.09D-04 BMatP= 6.40D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.87D-03

Coeff-Com: -0.107D-01 0.103D+00 0.304D+00 0.604D+00

Coeff-En: 0.000D+00 0.000D+00 0.105D+00 0.895D+00

Coeff: -0.106D-01 0.102D+00 0.303D+00 0.605D+00

Gap= 0.101 Goal= None Shift= 0.000

Gap= 0.054 Goal= None Shift= 0.000

RMSDP=4.71D-06 MaxDP=5.33D-04 DE=-1.26D-04 OVMax= 1.29D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.86D-06 CP: 9.99D-01 1.08D+00 8.15D-01 7.83D-01

E= -1914.19996116991 Delta-E= -0.000023877041 Rises=F Damp=F

DIIS: error= 5.99D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.19996116991 IErMin= 5 ErrMin= 5.99D-05

ErrMax= 5.99D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.34D-06 BMatP= 1.09D-04

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

Coeff-Com: -0.139D-02 0.981D-03 0.816D-01 0.258D+00 0.660D+00

Coeff: -0.139D-02 0.981D-03 0.816D-01 0.258D+00 0.660D+00

Gap= 0.101 Goal= None Shift= 0.000

Gap= 0.053 Goal= None Shift= 0.000

RMSDP=1.82D-06 MaxDP=1.47D-04 DE=-2.39D-05 OVMax= 6.50D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.47D-06 CP: 9.99D-01 1.08D+00 8.35D-01 8.27D-01 8.22D-01

E= -1914.19996242833 Delta-E= -0.000001258420 Rises=F Damp=F

DIIS: error= 2.98D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.19996242833 IErMin= 6 ErrMin= 2.98D-05

ErrMax= 2.98D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.18D-06 BMatP= 6.34D-06

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

Coeff-Com: 0.868D-03-0.165D-01 0.318D-03 0.591D-01 0.409D+00 0.547D+00

Coeff: 0.868D-03-0.165D-01 0.318D-03 0.591D-01 0.409D+00 0.547D+00

Gap= 0.101 Goal= None Shift= 0.000

Gap= 0.053 Goal= None Shift= 0.000

RMSDP=8.19D-07 MaxDP=6.92D-05 DE=-1.26D-06 OVMax= 4.60D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.50D-07 CP: 9.99D-01 1.08D+00 8.42D-01 8.38D-01 8.82D-01

CP: 6.69D-01

E= -1914.19996303309 Delta-E= -0.000000604756 Rises=F Damp=F

DIIS: error= 9.65D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.19996303309 IErMin= 7 ErrMin= 9.65D-06

ErrMax= 9.65D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.32D-07 BMatP= 2.18D-06

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

Coeff-Com: 0.457D-03-0.736D-02-0.403D-02 0.128D-01 0.148D+00 0.253D+00

Coeff-Com: 0.597D+00

Coeff: 0.457D-03-0.736D-02-0.403D-02 0.128D-01 0.148D+00 0.253D+00

Coeff: 0.597D+00

Gap= 0.101 Goal= None Shift= 0.000

Gap= 0.053 Goal= None Shift= 0.000

RMSDP=3.24D-07 MaxDP=2.98D-05 DE=-6.05D-07 OVMax= 1.11D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.72D-07 CP: 9.99D-01 1.08D+00 8.42D-01 8.45D-01 8.98D-01

CP: 7.65D-01 1.06D+00

E= -1914.19996310328 Delta-E= -0.000000070195 Rises=F Damp=F

DIIS: error= 6.39D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.19996310328 IErMin= 8 ErrMin= 6.39D-06

ErrMax= 6.39D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.76D-08 BMatP= 1.32D-07

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

Coeff-Com: -0.241D-03 0.540D-02-0.218D-02-0.264D-01-0.151D+00-0.164D+00

Coeff-Com: 0.322D+00 0.102D+01

Coeff: -0.241D-03 0.540D-02-0.218D-02-0.264D-01-0.151D+00-0.164D+00

Coeff: 0.322D+00 0.102D+01

Gap= 0.101 Goal= None Shift= 0.000

Gap= 0.053 Goal= None Shift= 0.000

RMSDP=3.52D-07 MaxDP=3.95D-05 DE=-7.02D-08 OVMax= 2.29D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.52D-07 CP: 9.99D-01 1.08D+00 8.43D-01 8.47D-01 9.20D-01

CP: 8.28D-01 1.58D+00 1.16D+00

E= -1914.19996316502 Delta-E= -0.000000061734 Rises=F Damp=F

DIIS: error= 4.32D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.19996316502 IErMin= 9 ErrMin= 4.32D-06

ErrMax= 4.32D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.10D-08 BMatP= 4.76D-08

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

Coeff-Com: -0.284D-03 0.556D-02-0.146D-03-0.205D-01-0.142D+00-0.181D+00

Coeff-Com: 0.126D-01 0.640D+00 0.685D+00

Coeff: -0.284D-03 0.556D-02-0.146D-03-0.205D-01-0.142D+00-0.181D+00

Coeff: 0.126D-01 0.640D+00 0.685D+00

Gap= 0.101 Goal= None Shift= 0.000

Gap= 0.053 Goal= None Shift= 0.000

RMSDP=2.01D-07 MaxDP=1.94D-05 DE=-6.17D-08 OVMax= 6.53D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 9.74D-08 CP: 9.99D-01 1.08D+00 8.43D-01 8.50D-01 9.27D-01

CP: 9.00D-01 1.77D+00 1.46D+00 9.69D-01

E= -1914.19996318054 Delta-E= -0.000000015525 Rises=F Damp=F

DIIS: error= 2.33D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.19996318054 IErMin=10 ErrMin= 2.33D-06

ErrMax= 2.33D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.62D-09 BMatP= 2.10D-08

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

Coeff-Com: -0.548D-04 0.791D-03 0.847D-03-0.210D-03-0.149D-01-0.298D-01

Coeff-Com: -0.111D+00-0.230D-01 0.390D+00 0.788D+00

Coeff: -0.548D-04 0.791D-03 0.847D-03-0.210D-03-0.149D-01-0.298D-01

Coeff: -0.111D+00-0.230D-01 0.390D+00 0.788D+00

Gap= 0.101 Goal= None Shift= 0.000

Gap= 0.053 Goal= None Shift= 0.000

RMSDP=8.49D-08 MaxDP=6.82D-06 DE=-1.55D-08 OVMax= 3.67D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 3.80D-08 CP: 9.99D-01 1.08D+00 8.43D-01 8.50D-01 9.29D-01

CP: 9.08D-01 1.85D+00 1.55D+00 1.31D+00 1.02D+00

E= -1914.19996318364 Delta-E= -0.000000003101 Rises=F Damp=F

DIIS: error= 1.15D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.19996318364 IErMin=11 ErrMin= 1.15D-06

ErrMax= 1.15D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.11D-10 BMatP= 4.62D-09

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

Coeff-Com: 0.186D-04-0.512D-03 0.452D-03 0.324D-02 0.157D-01 0.146D-01

Coeff-Com: -0.564D-01-0.112D+00 0.864D-01 0.362D+00 0.686D+00

Coeff: 0.186D-04-0.512D-03 0.452D-03 0.324D-02 0.157D-01 0.146D-01

Coeff: -0.564D-01-0.112D+00 0.864D-01 0.362D+00 0.686D+00

Gap= 0.101 Goal= None Shift= 0.000

Gap= 0.053 Goal= None Shift= 0.000

RMSDP=2.62D-08 MaxDP=1.17D-06 DE=-3.10D-09 OVMax= 9.90D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.74D-08 CP: 9.99D-01 1.08D+00 8.43D-01 8.50D-01 9.30D-01

CP: 9.08D-01 1.86D+00 1.58D+00 1.38D+00 1.14D+00

CP: 1.03D+00

E= -1914.19996318410 Delta-E= -0.000000000460 Rises=F Damp=F

DIIS: error= 5.78D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.19996318410 IErMin=12 ErrMin= 5.78D-07

ErrMax= 5.78D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.73D-10 BMatP= 7.11D-10

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

Coeff-Com: 0.201D-04-0.385D-03-0.572D-04 0.126D-02 0.964D-02 0.129D-01

Coeff-Com: 0.478D-02-0.396D-01-0.507D-01-0.590D-01 0.277D+00 0.844D+00

Coeff: 0.201D-04-0.385D-03-0.572D-04 0.126D-02 0.964D-02 0.129D-01

Coeff: 0.478D-02-0.396D-01-0.507D-01-0.590D-01 0.277D+00 0.844D+00

Gap= 0.101 Goal= None Shift= 0.000

Gap= 0.053 Goal= None Shift= 0.000

RMSDP=1.58D-08 MaxDP=7.06D-07 DE=-4.60D-10 OVMax= 5.99D-06

Cycle 13 Pass 1 IDiag 1:

RMSU= 9.23D-09 CP: 9.99D-01 1.08D+00 8.43D-01 8.50D-01 9.30D-01

CP: 9.08D-01 1.86D+00 1.59D+00 1.42D+00 1.22D+00

CP: 1.24D+00 1.25D+00

E= -1914.19996318426 Delta-E= -0.000000000154 Rises=F Damp=F

DIIS: error= 2.57D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1914.19996318426 IErMin=13 ErrMin= 2.57D-07

ErrMax= 2.57D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.85D-11 BMatP= 1.73D-10

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

Coeff-Com: 0.131D-05 0.350D-04-0.198D-03-0.666D-03-0.184D-02-0.208D-03

Coeff-Com: 0.224D-01 0.217D-01-0.440D-01-0.155D+00-0.119D+00 0.311D+00

Coeff-Com: 0.966D+00

Coeff: 0.131D-05 0.350D-04-0.198D-03-0.666D-03-0.184D-02-0.208D-03

Coeff: 0.224D-01 0.217D-01-0.440D-01-0.155D+00-0.119D+00 0.311D+00

Coeff: 0.966D+00

Gap= 0.101 Goal= None Shift= 0.000

Gap= 0.053 Goal= None Shift= 0.000

RMSDP=1.16D-08 MaxDP=7.59D-07 DE=-1.54D-10 OVMax= 3.56D-06

Cycle 14 Pass 1 IDiag 1:

RMSU= 4.57D-09 CP: 9.99D-01 1.08D+00 8.43D-01 8.50D-01 9.30D-01

CP: 9.07D-01 1.86D+00 1.59D+00 1.44D+00 1.24D+00

CP: 1.38D+00 1.66D+00 1.29D+00

E= -1914.19996318426 Delta-E= -0.000000000006 Rises=F Damp=F

DIIS: error= 1.08D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1914.19996318426 IErMin=14 ErrMin= 1.08D-07

ErrMax= 1.08D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.86D-11 BMatP= 4.85D-11

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

Coeff-Com: -0.399D-05 0.112D-03-0.103D-03-0.679D-03-0.335D-02-0.319D-02

Coeff-Com: 0.121D-01 0.211D-01-0.137D-01-0.755D-01-0.128D+00-0.148D-01

Coeff-Com: 0.560D+00 0.646D+00

Coeff: -0.399D-05 0.112D-03-0.103D-03-0.679D-03-0.335D-02-0.319D-02

Coeff: 0.121D-01 0.211D-01-0.137D-01-0.755D-01-0.128D+00-0.148D-01

Coeff: 0.560D+00 0.646D+00

Gap= 0.101 Goal= None Shift= 0.000

Gap= 0.053 Goal= None Shift= 0.000

RMSDP=4.55D-09 MaxDP=2.99D-07 DE=-6.37D-12 OVMax= 1.69D-06

Error on total polarization charges = 0.07936

SCF Done: E(UB3LYP) = -1914.19996318 A.U. after 14 cycles

NFock= 14 Conv=0.45D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7880 S= 0.5188

<L.S>= 0.000000000000E+00

KE= 1.906233053361D+03 PE=-1.515279852372D+04 EE= 5.963159272774D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.35

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7880, after 0.7512

Leave Link 502 at Sun Aug 18 13:54:14 2019, MaxMem= 2013265920 cpu: 2588.5

(Enter /home/kira/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

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

GePol: Maximum number of non-zero 1st derivatives = 191

Leave Link 701 at Sun Aug 18 13:54:31 2019, MaxMem= 2013265920 cpu: 139.8

(Enter /home/kira/g09/l702.exe)

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

Leave Link 702 at Sun Aug 18 13:54:31 2019, MaxMem= 2013265920 cpu: 0.2

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

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

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

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Sun Aug 18 13:55:10 2019, MaxMem= 2013265920 cpu: 307.5

(Enter /home/kira/g09/l716.exe)

Dipole =-1.53495925D-14 1.33226763D-13-1.31130543D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.002653233 -0.001299904 0.000245876

2 6 0.002118873 0.001026676 -0.000921545

3 7 -0.000000000 0.000922798 0.000123468

4 6 -0.002118873 0.001026676 -0.000921545

5 6 0.002653233 -0.001299904 0.000245876

6 6 0.002489762 0.000821180 -0.000015605

7 6 0.000812336 0.001049786 0.001091424

8 7 0.000280180 0.000000000 -0.000478694

9 6 0.000812336 -0.001049786 0.001091424

10 6 -0.000785966 -0.000539867 -0.000259844

11 6 -0.000785966 0.000539867 -0.000259844

12 6 -0.002489762 0.000821180 -0.000015605

13 6 -0.000812336 0.001049786 0.001091424

14 6 0.000785966 0.000539867 -0.000259844

15 6 0.000785966 -0.000539867 -0.000259844

16 6 -0.000812336 -0.001049786 0.001091424

17 7 -0.000280180 0.000000000 -0.000478694

18 6 -0.002489762 -0.000821180 -0.000015605

19 6 0.002118873 -0.001026676 -0.000921545

20 6 -0.002653233 0.001299904 0.000245876

21 6 0.002653233 0.001299904 0.000245876

22 6 -0.002118873 -0.001026676 -0.000921545

23 7 0.000000000 -0.000922798 0.000123468

24 6 0.002489762 -0.000821180 -0.000015605

25 6 -0.001549521 -0.001267833 -0.000149393

26 6 -0.000006096 0.000995915 -0.000380163

27 6 -0.000022581 0.000077159 0.000070950

28 6 0.000015285 0.000015904 -0.000006297

29 6 0.000084516 -0.000021426 -0.000069834

30 6 0.000980592 -0.000116057 0.000356708

31 6 -0.000015285 0.000015904 -0.000006297

32 6 0.000022581 0.000077159 0.000070950

33 6 0.000006096 0.000995915 -0.000380163

34 6 0.001549521 -0.001267833 -0.000149393

35 6 -0.000980592 -0.000116057 0.000356708

36 6 -0.000084516 -0.000021426 -0.000069834

37 6 -0.001549521 0.001267833 -0.000149393

38 6 0.000980592 0.000116057 0.000356708

39 6 0.000084516 0.000021426 -0.000069834

40 6 0.000015285 -0.000015904 -0.000006297

41 6 -0.000022581 -0.000077159 0.000070950

42 6 -0.000006096 -0.000995915 -0.000380163

43 6 0.001549521 0.001267833 -0.000149393

44 6 -0.000980592 0.000116057 0.000356708

45 6 -0.000084516 0.000021426 -0.000069834

46 6 -0.000015285 -0.000015904 -0.000006297

47 6 0.000022581 -0.000077159 0.000070950

48 6 0.000006096 -0.000995915 -0.000380163

49 1 0.000341599 -0.000138045 0.000309361

50 1 -0.000341599 -0.000138045 0.000309361

51 1 -0.000108800 0.000194712 -0.000230081

52 1 -0.000108800 -0.000194712 -0.000230081

53 1 0.000108800 -0.000194712 -0.000230081

54 1 0.000108800 0.000194712 -0.000230081

55 1 0.000341599 0.000138045 0.000309361

56 1 -0.000341599 0.000138045 0.000309361

57 1 0.000293440 -0.000131762 0.000138907

58 1 0.000180878 0.000017039 -0.000032067

59 1 0.000024973 0.000025518 0.000004573

60 1 0.000013729 0.000184285 0.000035062

61 1 -0.000136066 0.000287636 -0.000120960

62 1 -0.000024973 0.000025518 0.000004573

63 1 -0.000180878 0.000017039 -0.000032067

64 1 -0.000293440 -0.000131762 0.000138907

65 1 0.000136066 0.000287636 -0.000120960

66 1 -0.000013729 0.000184285 0.000035062

67 1 -0.000136066 -0.000287636 -0.000120960

68 1 0.000013729 -0.000184285 0.000035062

69 1 0.000024973 -0.000025518 0.000004573

70 1 0.000180878 -0.000017039 -0.000032067

71 1 0.000293440 0.000131762 0.000138907

72 1 0.000136066 -0.000287636 -0.000120960

73 1 -0.000013729 -0.000184285 0.000035062

74 1 -0.000024973 -0.000025518 0.000004573

75 1 -0.000180878 -0.000017039 -0.000032067

76 1 -0.000293440 0.000131762 0.000138907

77 1 0.000000000 0.000778856 0.000221077

78 1 -0.000000000 -0.000778856 0.000221077

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

Cartesian Forces: Max 0.002653233 RMS 0.000760550

Leave Link 716 at Sun Aug 18 13:55:10 2019, MaxMem= 2013265920 cpu: 0.2

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

Internal Forces: Max 0.002430931 RMS 0.000481872

Search for a local minimum.

Step number 2 out of a maximum of 452

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

RMS Force = .48187D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 1 2

DE= -1.59D-03 DEPred=-1.64D-03 R= 9.67D-01

TightC=F SS= 1.41D+00 RLast= 2.82D-01 DXNew= 5.0454D-01 8.4514D-01

Trust test= 9.67D-01 RLast= 2.82D-01 DXMaxT set to 5.05D-01

ITU= 1 0

Use linear search instead of GDIIS.

Eigenvalues --- 0.00861 0.00861 0.00861 0.00902 0.01643

Eigenvalues --- 0.01654 0.01666 0.01667 0.01690 0.01690

Eigenvalues --- 0.01713 0.01713 0.01713 0.01713 0.01720

Eigenvalues --- 0.01733 0.01814 0.01821 0.01825 0.01857

Eigenvalues --- 0.01863 0.01869 0.01893 0.01905 0.01906

Eigenvalues --- 0.01945 0.01968 0.01998 0.02008 0.02017

Eigenvalues --- 0.02019 0.02025 0.02029 0.02041 0.02050

Eigenvalues --- 0.02063 0.02072 0.02081 0.02096 0.02099

Eigenvalues --- 0.02099 0.02099 0.02099 0.02130 0.02132

Eigenvalues --- 0.02132 0.02132 0.02140 0.02140 0.02140

Eigenvalues --- 0.02140 0.02161 0.02161 0.02161 0.02165

Eigenvalues --- 0.02165 0.02165 0.02165 0.02171 0.02171

Eigenvalues --- 0.02171 0.02171 0.02174 0.02175 0.02175

Eigenvalues --- 0.02175 0.02176 0.02176 0.02176 0.02176

Eigenvalues --- 0.02213 0.02213 0.02220 0.02225 0.02226

Eigenvalues --- 0.15974 0.15991 0.15991 0.15992 0.15992

Eigenvalues --- 0.15995 0.15995 0.15995 0.15995 0.15997

Eigenvalues --- 0.15998 0.15998 0.15998 0.15998 0.15998

Eigenvalues --- 0.15998 0.15998 0.15999 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16036

Eigenvalues --- 0.21999 0.21999 0.21999 0.21999 0.22000

Eigenvalues --- 0.22000 0.22000 0.22000 0.22782 0.22797

Eigenvalues --- 0.22802 0.22816 0.23434 0.23478 0.23478

Eigenvalues --- 0.23478 0.23541 0.23809 0.24474 0.24741

Eigenvalues --- 0.24811 0.24911 0.24938 0.24978 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.28326 0.32178 0.33146 0.33146

Eigenvalues --- 0.33146 0.34571 0.34600 0.35385 0.35400

Eigenvalues --- 0.35400 0.35400 0.35400 0.35400 0.35400

Eigenvalues --- 0.35400 0.35405 0.35405 0.35405 0.35405

Eigenvalues --- 0.35452 0.35452 0.35452 0.35456 0.35461

Eigenvalues --- 0.35461 0.35461 0.35516 0.36087 0.36108

Eigenvalues --- 0.36108 0.36108 0.36232 0.36232 0.36232

Eigenvalues --- 0.36238 0.36737 0.36879 0.37381 0.37411

Eigenvalues --- 0.38765 0.39538 0.40699 0.41985 0.41985

Eigenvalues --- 0.41985 0.42166 0.42166 0.42166 0.42166

Eigenvalues --- 0.42502 0.43287 0.43539 0.44397 0.44420

Eigenvalues --- 0.44677 0.44770 0.45373 0.45482 0.45562

Eigenvalues --- 0.45632 0.45767 0.45854 0.45854 0.45854

Eigenvalues --- 0.45854 0.46151 0.46151 0.46151 0.46213

Eigenvalues --- 0.46306 0.46645 0.46645 0.46645 0.46645

Eigenvalues --- 0.46835 0.46835 0.46835 0.46863 0.47582

Eigenvalues --- 0.48581 0.48633 0.49754 0.49860 0.50661

Eigenvalues --- 0.51511 0.53098 0.54860

RFO step: Lambda=-8.59507256D-04 EMin= 8.61370080D-03

Quartic linear search produced a step of 0.03802.

Iteration 1 RMS(Cart)= 0.04656550 RMS(Int)= 0.00049213

Iteration 2 RMS(Cart)= 0.00093972 RMS(Int)= 0.00004174

Iteration 3 RMS(Cart)= 0.00000029 RMS(Int)= 0.00004174

ITry= 1 IFail=0 DXMaxC= 2.48D-01 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.72D-08 for atom 54.

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

(Linear) (Quad) (Total)

R1 2.70038 -0.00138 -0.00029 -0.00523 -0.00550 2.69488

R2 2.58823 0.00204 0.00009 0.00506 0.00522 2.59345

R3 2.03653 -0.00028 -0.00003 -0.00097 -0.00099 2.03553

R4 2.59205 -0.00002 -0.00033 -0.00243 -0.00280 2.58924

R5 2.66254 0.00243 0.00062 0.00944 0.01006 2.67259

R6 2.59205 -0.00002 -0.00033 -0.00243 -0.00280 2.58924

R7 1.91497 -0.00079 0.00009 -0.00119 -0.00109 1.91387

R8 2.70038 -0.00138 -0.00029 -0.00523 -0.00550 2.69488

R9 2.66254 0.00243 0.00062 0.00944 0.01006 2.67259

R10 2.03653 -0.00028 -0.00003 -0.00097 -0.00099 2.03553

R11 2.66118 0.00127 0.00005 0.00328 0.00333 2.66451

R12 2.80795 -0.00004 -0.00049 -0.00327 -0.00376 2.80419

R13 2.57976 0.00128 -0.00015 0.00157 0.00136 2.58112

R14 2.75265 -0.00061 -0.00012 -0.00244 -0.00254 2.75012

R15 2.57976 0.00128 -0.00015 0.00157 0.00136 2.58112

R16 2.75265 -0.00061 -0.00012 -0.00244 -0.00254 2.75012

R17 2.66118 0.00127 0.00005 0.00328 0.00333 2.66451

R18 2.55872 0.00099 -0.00006 0.00153 0.00154 2.56026

R19 2.03804 -0.00018 -0.00004 -0.00077 -0.00081 2.03723

R20 2.03804 -0.00018 -0.00004 -0.00077 -0.00081 2.03723

R21 2.66118 0.00127 0.00005 0.00328 0.00333 2.66451

R22 2.80795 -0.00004 -0.00049 -0.00327 -0.00376 2.80419

R23 2.75265 -0.00061 -0.00012 -0.00244 -0.00254 2.75012

R24 2.57976 0.00128 -0.00015 0.00157 0.00136 2.58112

R25 2.55872 0.00099 -0.00006 0.00153 0.00154 2.56026

R26 2.03804 -0.00018 -0.00004 -0.00077 -0.00081 2.03723

R27 2.75265 -0.00061 -0.00012 -0.00244 -0.00254 2.75012

R28 2.03804 -0.00018 -0.00004 -0.00077 -0.00081 2.03723

R29 2.57976 0.00128 -0.00015 0.00157 0.00136 2.58112

R30 2.66118 0.00127 0.00005 0.00328 0.00333 2.66451

R31 2.66254 0.00243 0.00062 0.00944 0.01006 2.67259

R32 2.80795 -0.00004 -0.00049 -0.00327 -0.00376 2.80419

R33 2.70038 -0.00138 -0.00029 -0.00523 -0.00550 2.69488

R34 2.59205 -0.00002 -0.00033 -0.00243 -0.00280 2.58924

R35 2.58823 0.00204 0.00009 0.00506 0.00522 2.59345

R36 2.03653 -0.00028 -0.00003 -0.00097 -0.00099 2.03553

R37 2.70038 -0.00138 -0.00029 -0.00523 -0.00550 2.69488

R38 2.03653 -0.00028 -0.00003 -0.00097 -0.00099 2.03553

R39 2.59205 -0.00002 -0.00033 -0.00243 -0.00280 2.58924

R40 2.66254 0.00243 0.00062 0.00944 0.01006 2.67259

R41 1.91497 -0.00079 0.00009 -0.00119 -0.00109 1.91387

R42 2.80795 -0.00004 -0.00049 -0.00327 -0.00376 2.80419

R43 2.64561 0.00097 0.00000 0.00230 0.00231 2.64791

R44 2.64573 0.00094 -0.00000 0.00219 0.00219 2.64792

R45 2.62934 0.00021 -0.00011 -0.00024 -0.00035 2.62898

R46 2.04921 -0.00029 -0.00001 -0.00092 -0.00093 2.04828

R47 2.63515 -0.00012 0.00002 -0.00022 -0.00020 2.63495

R48 2.04944 0.00004 -0.00003 -0.00009 -0.00012 2.04932

R49 2.63558 -0.00012 0.00003 -0.00016 -0.00014 2.63545

R50 2.04969 0.00004 -0.00002 -0.00002 -0.00004 2.04965

R51 2.62875 0.00021 -0.00012 -0.00027 -0.00038 2.62837

R52 2.04944 0.00004 -0.00003 -0.00009 -0.00012 2.04932

R53 2.04906 -0.00028 -0.00001 -0.00087 -0.00088 2.04818

R54 2.63515 -0.00012 0.00002 -0.00022 -0.00020 2.63495

R55 2.63558 -0.00012 0.00003 -0.00016 -0.00014 2.63545

R56 2.04969 0.00004 -0.00002 -0.00002 -0.00004 2.04965

R57 2.62934 0.00021 -0.00011 -0.00024 -0.00035 2.62898

R58 2.04944 0.00004 -0.00003 -0.00009 -0.00012 2.04932

R59 2.64561 0.00097 0.00000 0.00230 0.00231 2.64791

R60 2.04921 -0.00029 -0.00001 -0.00092 -0.00093 2.04828

R61 2.64573 0.00094 -0.00000 0.00219 0.00219 2.64792

R62 2.62875 0.00021 -0.00012 -0.00027 -0.00038 2.62837

R63 2.04906 -0.00028 -0.00001 -0.00087 -0.00088 2.04818

R64 2.04944 0.00004 -0.00003 -0.00009 -0.00012 2.04932

R65 2.64573 0.00094 -0.00000 0.00219 0.00219 2.64792

R66 2.64561 0.00097 0.00000 0.00230 0.00231 2.64791

R67 2.62875 0.00021 -0.00012 -0.00027 -0.00038 2.62837

R68 2.04906 -0.00028 -0.00001 -0.00087 -0.00088 2.04818

R69 2.63558 -0.00012 0.00003 -0.00016 -0.00014 2.63545

R70 2.04944 0.00004 -0.00003 -0.00009 -0.00012 2.04932

R71 2.63515 -0.00012 0.00002 -0.00022 -0.00020 2.63495

R72 2.04969 0.00004 -0.00002 -0.00002 -0.00004 2.04965

R73 2.62934 0.00021 -0.00011 -0.00024 -0.00035 2.62898

R74 2.04944 0.00004 -0.00003 -0.00009 -0.00012 2.04932

R75 2.04921 -0.00029 -0.00001 -0.00092 -0.00093 2.04828

R76 2.64573 0.00094 -0.00000 0.00219 0.00219 2.64792

R77 2.64561 0.00097 0.00000 0.00230 0.00231 2.64791

R78 2.62875 0.00021 -0.00012 -0.00027 -0.00038 2.62837

R79 2.04906 -0.00028 -0.00001 -0.00087 -0.00088 2.04818

R80 2.63558 -0.00012 0.00003 -0.00016 -0.00014 2.63545

R81 2.04944 0.00004 -0.00003 -0.00009 -0.00012 2.04932

R82 2.63515 -0.00012 0.00002 -0.00022 -0.00020 2.63495

R83 2.04969 0.00004 -0.00002 -0.00002 -0.00004 2.04965

R84 2.62934 0.00021 -0.00011 -0.00024 -0.00035 2.62898

R85 2.04944 0.00004 -0.00003 -0.00009 -0.00012 2.04932

R86 2.04921 -0.00029 -0.00001 -0.00092 -0.00093 2.04828

A1 1.88324 0.00006 -0.00020 -0.00064 -0.00088 1.88237

A2 2.18134 0.00018 0.00012 0.00178 0.00191 2.18325

A3 2.21846 -0.00024 0.00008 -0.00124 -0.00115 2.21731

A4 1.86857 -0.00058 0.00039 -0.00033 0.00001 1.86857

A5 2.20710 0.00001 -0.00024 -0.00051 -0.00059 2.20651

A6 2.20752 0.00057 -0.00015 0.00085 0.00055 2.20807

A7 1.92108 0.00103 -0.00038 0.00171 0.00131 1.92239

A8 2.18089 -0.00051 0.00019 -0.00070 -0.00054 2.18036

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D3 -3.11797 0.00032 0.00003 0.01692 0.01694 -3.10103

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D136 0.00495 0.00007 0.00001 0.00343 0.00344 0.00838

D137 0.00773 0.00003 0.00022 0.00257 0.00280 0.01053

D138 -3.13689 0.00007 0.00002 0.00335 0.00338 -3.13351

D139 -3.13375 0.00003 0.00022 0.00260 0.00283 -3.13093

D140 0.00481 0.00007 0.00002 0.00339 0.00341 0.00822

D141 -0.01504 -0.00006 -0.00044 -0.00557 -0.00600 -0.02104

D142 3.14089 0.00008 -0.00019 0.00258 0.00240 -3.13990

D143 3.12957 -0.00011 -0.00024 -0.00634 -0.00658 3.12299

D144 0.00231 0.00004 0.00002 0.00181 0.00182 0.00413

D145 -0.00765 -0.00003 -0.00021 -0.00273 -0.00295 -0.01060

D146 3.13654 -0.00007 -0.00000 -0.00346 -0.00347 3.13307

D147 3.13405 -0.00003 -0.00022 -0.00270 -0.00292 3.13113

D148 -0.00495 -0.00007 -0.00001 -0.00343 -0.00344 -0.00838

D149 -0.00773 -0.00003 -0.00022 -0.00257 -0.00280 -0.01053

D150 3.13689 -0.00007 -0.00002 -0.00335 -0.00338 3.13351

D151 3.13375 -0.00003 -0.00022 -0.00260 -0.00283 3.13093

D152 -0.00481 -0.00007 -0.00002 -0.00339 -0.00341 -0.00822

D153 0.01573 0.00005 0.00043 0.00501 0.00544 0.02116

D154 3.14041 -0.00008 0.00019 -0.00268 -0.00249 3.13792

D155 -3.12845 0.00010 0.00022 0.00573 0.00595 -3.12250

D156 -0.00376 -0.00004 -0.00002 -0.00196 -0.00198 -0.00574

D157 3.13377 -0.00004 -0.00019 -0.00315 -0.00334 3.13043

D158 -0.00841 -0.00002 -0.00022 -0.00200 -0.00222 -0.01063

D159 0.00900 0.00009 0.00005 0.00450 0.00455 0.01355

D160 -3.13317 0.00012 0.00002 0.00565 0.00567 -3.12750

D161 3.13405 -0.00002 -0.00024 -0.00213 -0.00237 3.13168

D162 0.00672 0.00012 0.00001 0.00597 0.00598 0.01270

D163 -0.00696 -0.00004 -0.00022 -0.00327 -0.00349 -0.01045

D164 -3.13429 0.00010 0.00003 0.00483 0.00486 -3.12943

D165 0.01504 0.00006 0.00044 0.00557 0.00600 0.02104

D166 -3.12957 0.00011 0.00024 0.00634 0.00658 -3.12299

D167 -3.14089 -0.00008 0.00019 -0.00258 -0.00240 3.13990

D168 -0.00231 -0.00004 -0.00002 -0.00181 -0.00182 -0.00413

D169 3.13405 -0.00002 -0.00024 -0.00213 -0.00237 3.13168

D170 0.00672 0.00012 0.00001 0.00597 0.00598 0.01270

D171 -0.00696 -0.00004 -0.00022 -0.00327 -0.00349 -0.01045

D172 -3.13429 0.00010 0.00003 0.00483 0.00486 -3.12943

D173 3.13377 -0.00004 -0.00019 -0.00315 -0.00334 3.13043

D174 0.00900 0.00009 0.00005 0.00450 0.00455 0.01355

D175 -0.00841 -0.00002 -0.00022 -0.00200 -0.00222 -0.01063

D176 -3.13317 0.00012 0.00002 0.00565 0.00567 -3.12750

D177 0.01504 0.00006 0.00044 0.00557 0.00600 0.02104

D178 -3.12957 0.00011 0.00024 0.00634 0.00658 -3.12299

D179 -3.14089 -0.00008 0.00019 -0.00258 -0.00240 3.13990

D180 -0.00231 -0.00004 -0.00002 -0.00181 -0.00182 -0.00413

D181 -0.00773 -0.00003 -0.00022 -0.00257 -0.00280 -0.01053

D182 3.13375 -0.00003 -0.00022 -0.00260 -0.00283 3.13093

D183 3.13689 -0.00007 -0.00002 -0.00335 -0.00338 3.13351

D184 -0.00481 -0.00007 -0.00002 -0.00339 -0.00341 -0.00822

D185 -0.00765 -0.00003 -0.00021 -0.00273 -0.00295 -0.01060

D186 3.13654 -0.00007 -0.00000 -0.00346 -0.00347 3.13307

D187 3.13405 -0.00003 -0.00022 -0.00270 -0.00292 3.13113

D188 -0.00495 -0.00007 -0.00001 -0.00343 -0.00344 -0.00838

D189 0.01573 0.00005 0.00043 0.00501 0.00544 0.02116

D190 3.14041 -0.00008 0.00019 -0.00268 -0.00249 3.13792

D191 -3.12845 0.00010 0.00022 0.00573 0.00595 -3.12250

D192 -0.00376 -0.00004 -0.00002 -0.00196 -0.00198 -0.00574

D193 -3.13405 0.00002 0.00024 0.00213 0.00237 -3.13168

D194 -0.00672 -0.00012 -0.00001 -0.00597 -0.00598 -0.01270

D195 0.00696 0.00004 0.00022 0.00327 0.00349 0.01045

D196 3.13429 -0.00010 -0.00003 -0.00483 -0.00486 3.12943

D197 -3.13377 0.00004 0.00019 0.00315 0.00334 -3.13043

D198 -0.00900 -0.00009 -0.00005 -0.00450 -0.00455 -0.01355

D199 0.00841 0.00002 0.00022 0.00200 0.00222 0.01063

D200 3.13317 -0.00012 -0.00002 -0.00565 -0.00567 3.12750

D201 -0.01504 -0.00006 -0.00044 -0.00557 -0.00600 -0.02104

D202 3.12957 -0.00011 -0.00024 -0.00634 -0.00658 3.12299

D203 3.14089 0.00008 -0.00019 0.00258 0.00240 -3.13990

D204 0.00231 0.00004 0.00002 0.00181 0.00182 0.00413

D205 0.00773 0.00003 0.00022 0.00257 0.00280 0.01053

D206 -3.13375 0.00003 0.00022 0.00260 0.00283 -3.13093

D207 -3.13689 0.00007 0.00002 0.00335 0.00338 -3.13351

D208 0.00481 0.00007 0.00002 0.00339 0.00341 0.00822

D209 0.00765 0.00003 0.00021 0.00273 0.00295 0.01060

D210 -3.13654 0.00007 0.00000 0.00346 0.00347 -3.13307

D211 -3.13405 0.00003 0.00022 0.00270 0.00292 -3.13113

D212 0.00495 0.00007 0.00001 0.00343 0.00344 0.00838

D213 -0.01573 -0.00005 -0.00043 -0.00501 -0.00544 -0.02116

D214 -3.14041 0.00008 -0.00019 0.00268 0.00249 -3.13792

D215 3.12845 -0.00010 -0.00022 -0.00573 -0.00595 3.12250

D216 0.00376 0.00004 0.00002 0.00196 0.00198 0.00574

Item Value Threshold Converged?

Maximum Force 0.002431 0.000450 NO

RMS Force 0.000482 0.000300 NO

Maximum Displacement 0.248055 0.001800 NO

RMS Displacement 0.046658 0.001200 NO

Predicted change in Energy=-4.471449D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Aug 18 13:55:10 2019, MaxMem= 2013265920 cpu: 1.4

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

Stoichiometry C44H30N4(1+,2)

Framework group C2V[SGV(H2N2),SGV'(N2),X(C44H28)]

Deg. of freedom 59

Full point group C2V NOp 4

RotChk: IX=0 Diff= 9.57D-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 -0.686198 4.215219 0.290667

2 6 0 -1.123368 2.875015 0.075231

3 7 0 0.000000 2.097125 -0.026219

4 6 0 1.123368 2.875015 0.075231

5 6 0 0.686198 4.215219 0.290667

6 6 0 2.463945 2.432037 -0.007237

7 6 0 2.880058 1.087468 -0.091348

8 7 0 2.060540 -0.000000 0.015455

9 6 0 2.880058 -1.087468 -0.091348

10 6 0 4.257361 -0.677416 -0.321109

11 6 0 4.257361 0.677416 -0.321109

12 6 0 -2.463945 2.432037 -0.007237

13 6 0 -2.880058 1.087468 -0.091348

14 6 0 -4.257361 0.677416 -0.321109

15 6 0 -4.257361 -0.677416 -0.321109

16 6 0 -2.880058 -1.087468 -0.091348

17 7 0 -2.060540 0.000000 0.015455

18 6 0 -2.463945 -2.432037 -0.007237

19 6 0 -1.123368 -2.875015 0.075231

20 6 0 -0.686198 -4.215219 0.290667

21 6 0 0.686198 -4.215219 0.290667

22 6 0 1.123368 -2.875015 0.075231

23 7 0 -0.000000 -2.097125 -0.026219

24 6 0 2.463945 -2.432037 -0.007237

25 6 0 3.510359 3.484157 0.000395

26 6 0 3.542199 4.461584 -1.003113

27 6 0 4.534113 5.437031 -0.996991

28 6 0 5.485938 5.461591 0.021660

29 6 0 5.451193 4.498559 1.029788

30 6 0 4.476864 3.506097 1.014694

31 6 0 -5.485938 5.461591 0.021660

32 6 0 -4.534113 5.437031 -0.996991

33 6 0 -3.542199 4.461584 -1.003113

34 6 0 -3.510359 3.484157 0.000395

35 6 0 -4.476864 3.506097 1.014694

36 6 0 -5.451193 4.498559 1.029788

37 6 0 3.510359 -3.484157 0.000395

38 6 0 4.476864 -3.506097 1.014694

39 6 0 5.451193 -4.498559 1.029788

40 6 0 5.485938 -5.461591 0.021660

41 6 0 4.534113 -5.437031 -0.996991

42 6 0 3.542199 -4.461584 -1.003113

43 6 0 -3.510359 -3.484157 0.000395

44 6 0 -4.476864 -3.506097 1.014694

45 6 0 -5.451193 -4.498559 1.029788

46 6 0 -5.485938 -5.461591 0.021660

47 6 0 -4.534113 -5.437031 -0.996991

48 6 0 -3.542199 -4.461584 -1.003113

49 1 0 -1.335087 5.060679 0.446909

50 1 0 1.335087 5.060679 0.446909

51 1 0 5.096086 -1.334662 -0.484721

52 1 0 5.096086 1.334662 -0.484721

53 1 0 -5.096086 1.334662 -0.484721

54 1 0 -5.096086 -1.334662 -0.484721

55 1 0 -1.335087 -5.060679 0.446909

56 1 0 1.335087 -5.060679 0.446909

57 1 0 2.804315 4.440389 -1.796793

58 1 0 4.561558 6.178880 -1.787525

59 1 0 6.252618 6.228762 0.029931

60 1 0 6.184676 4.517824 1.828332

61 1 0 4.448414 2.758333 1.798766

62 1 0 -6.252618 6.228762 0.029931

63 1 0 -4.561558 6.178880 -1.787525

64 1 0 -2.804315 4.440389 -1.796793

65 1 0 -4.448414 2.758333 1.798766

66 1 0 -6.184676 4.517824 1.828332

67 1 0 4.448414 -2.758333 1.798766

68 1 0 6.184676 -4.517824 1.828332

69 1 0 6.252618 -6.228762 0.029931

70 1 0 4.561558 -6.178880 -1.787525

71 1 0 2.804315 -4.440389 -1.796793

72 1 0 -4.448414 -2.758333 1.798766

73 1 0 -6.184676 -4.517824 1.828332

74 1 0 -6.252618 -6.228762 0.029931

75 1 0 -4.561558 -6.178880 -1.787525

76 1 0 -2.804315 -4.440389 -1.796793

77 1 0 0.000000 1.091468 -0.146108

78 1 0 -0.000000 -1.091468 -0.146108

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

Rotational constants (GHZ): 0.0590281 0.0583952 0.0302702

Leave Link 202 at Sun Aug 18 13:55:10 2019, MaxMem= 2013265920 cpu: 0.1

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

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

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

There are 261 symmetry adapted cartesian basis functions of A1 symmetry.

There are 240 symmetry adapted cartesian basis functions of A2 symmetry.

There are 249 symmetry adapted cartesian basis functions of B1 symmetry.

There are 252 symmetry adapted cartesian basis functions of B2 symmetry.

There are 248 symmetry adapted basis functions of A1 symmetry.

There are 229 symmetry adapted basis functions of A2 symmetry.

There are 237 symmetry adapted basis functions of B1 symmetry.

There are 240 symmetry adapted basis functions of B2 symmetry.

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

161 alpha electrons 160 beta electrons

nuclear repulsion energy 5366.9573397745 Hartrees.

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

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

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

NAtoms= 78 NActive= 78 NUniq= 21 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=T Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2125095416 Hartrees.

Nuclear repulsion after empirical dispersion term = 5366.7448302329 Hartrees.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 78

GePol: Total number of spheres = 78

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

GePol: Number of points = 5730

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.46D-08

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 250

GePol: Fraction of low-weight points (<1% of avg) = 4.36%

GePol: Cavity surface area = 611.618 Ang\*\*2

GePol: Cavity volume = 625.334 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0021380032 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5366.7426922297 Hartrees.

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(Enter /home/kira/g09/l302.exe)

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

NBasis= 954 RedAO= T EigKep= 6.27D-05 NBF= 248 229 237 240

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 248 229 237 240

Precomputing XC quadrature grid using

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

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

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

Leave Link 302 at Sun Aug 18 13:55:11 2019, MaxMem= 2013265920 cpu: 10.1

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

DipDrv: MaxL=1.

Leave Link 303 at Sun Aug 18 13:55:12 2019, MaxMem= 2013265920 cpu: 1.3

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

Initial guess from the checkpoint file: "TPPcation.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) (B1) (A1) (B2) (A2) (A1) (B1) (A2) (B2)

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

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The electronic state of the initial guess is 2-A1.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7881 S= 0.5189

Generating alternative initial guess.

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -1914.09226201232

Leave Link 401 at Sun Aug 18 13:55:18 2019, MaxMem= 2013265920 cpu: 47.2

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3049894 IEndB= 3049894 NGot= 2013265920 MDV= 2011237673

LenX= 2011237673 LenY= 2010232667

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

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

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

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

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

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 98498700.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.22D-15 for 5696.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.63D-15 for 2382 1514.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.44D-15 for 5725.

Iteration 1 A^-1\*A deviation from orthogonality is 1.06D-14 for 2940 2938.

E= -1914.18506752077

DIIS: error= 3.56D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.18506752077 IErMin= 1 ErrMin= 3.56D-03

ErrMax= 3.56D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.91D-02 BMatP= 2.91D-02

IDIUse=3 WtCom= 9.64D-01 WtEn= 3.56D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.504 Goal= None Shift= 0.000

Gap= 0.515 Goal= None Shift= 0.000

GapD= 0.504 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=1.27D-04 MaxDP=4.14D-03 OVMax= 1.84D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.26D-04 CP: 9.99D-01

E= -1914.20013252934 Delta-E= -0.015065008570 Rises=F Damp=F

DIIS: error= 4.77D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.20013252934 IErMin= 2 ErrMin= 4.77D-04

ErrMax= 4.77D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.05D-04 BMatP= 2.91D-02

IDIUse=3 WtCom= 9.95D-01 WtEn= 4.77D-03

Coeff-Com: -0.614D-01 0.106D+01

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

Coeff: -0.611D-01 0.106D+01

Gap= 0.100 Goal= None Shift= 0.000

Gap= 0.054 Goal= None Shift= 0.000

RMSDP=2.43D-05 MaxDP=8.32D-04 DE=-1.51D-02 OVMax= 4.46D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.21D-05 CP: 9.99D-01 1.08D+00

E= -1914.20033155388 Delta-E= -0.000199024536 Rises=F Damp=F

DIIS: error= 3.09D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.20033155388 IErMin= 3 ErrMin= 3.09D-04

ErrMax= 3.09D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.48D-04 BMatP= 5.05D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.09D-03

Coeff-Com: -0.386D-01 0.510D+00 0.528D+00

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

Coeff: -0.385D-01 0.509D+00 0.530D+00

Gap= 0.099 Goal= None Shift= 0.000

Gap= 0.055 Goal= None Shift= 0.000

RMSDP=1.18D-05 MaxDP=7.38D-04 DE=-1.99D-04 OVMax= 3.09D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 9.22D-06 CP: 9.99D-01 1.09D+00 6.75D-01

E= -1914.20040004561 Delta-E= -0.000068491730 Rises=F Damp=F

DIIS: error= 1.55D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.20040004561 IErMin= 4 ErrMin= 1.55D-04

ErrMax= 1.55D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.48D-05 BMatP= 3.48D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.55D-03

Coeff-Com: -0.109D-01 0.111D+00 0.309D+00 0.591D+00

Coeff-En: 0.000D+00 0.000D+00 0.147D+00 0.853D+00

Coeff: -0.108D-01 0.111D+00 0.309D+00 0.591D+00

Gap= 0.099 Goal= None Shift= 0.000

Gap= 0.055 Goal= None Shift= 0.000

RMSDP=4.86D-06 MaxDP=3.18D-04 DE=-6.85D-05 OVMax= 1.41D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.93D-06 CP: 9.99D-01 1.10D+00 7.71D-01 6.58D-01

E= -1914.20041453056 Delta-E= -0.000014484951 Rises=F Damp=F

DIIS: error= 4.06D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.20041453056 IErMin= 5 ErrMin= 4.06D-05

ErrMax= 4.06D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.22D-06 BMatP= 6.48D-05

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

Coeff-Com: -0.211D-02 0.963D-02 0.103D+00 0.282D+00 0.608D+00

Coeff: -0.211D-02 0.963D-02 0.103D+00 0.282D+00 0.608D+00

Gap= 0.099 Goal= None Shift= 0.000

Gap= 0.055 Goal= None Shift= 0.000

RMSDP=1.64D-06 MaxDP=1.32D-04 DE=-1.45D-05 OVMax= 5.70D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.17D-06 CP: 9.99D-01 1.10D+00 7.70D-01 7.45D-01 7.27D-01

E= -1914.20041531854 Delta-E= -0.000000787983 Rises=F Damp=F

DIIS: error= 2.25D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.20041531854 IErMin= 6 ErrMin= 2.25D-05

ErrMax= 2.25D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.28D-06 BMatP= 4.22D-06

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

Coeff-Com: 0.757D-03-0.164D-01 0.447D-02 0.623D-01 0.388D+00 0.561D+00

Coeff: 0.757D-03-0.164D-01 0.447D-02 0.623D-01 0.388D+00 0.561D+00

Gap= 0.099 Goal= None Shift= 0.000

Gap= 0.055 Goal= None Shift= 0.000

RMSDP=7.52D-07 MaxDP=5.32D-05 DE=-7.88D-07 OVMax= 2.61D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 3.84D-07 CP: 9.99D-01 1.10D+00 7.84D-01 7.38D-01 8.21D-01

CP: 5.77D-01

E= -1914.20041562366 Delta-E= -0.000000305115 Rises=F Damp=F

DIIS: error= 5.32D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.20041562366 IErMin= 7 ErrMin= 5.32D-06

ErrMax= 5.32D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.32D-08 BMatP= 1.28D-06

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

Coeff-Com: 0.528D-03-0.968D-02-0.250D-02 0.215D-01 0.189D+00 0.318D+00

Coeff-Com: 0.484D+00

Coeff: 0.528D-03-0.968D-02-0.250D-02 0.215D-01 0.189D+00 0.318D+00

Coeff: 0.484D+00

Gap= 0.099 Goal= None Shift= 0.000

Gap= 0.055 Goal= None Shift= 0.000

RMSDP=1.89D-07 MaxDP=8.71D-06 DE=-3.05D-07 OVMax= 7.07D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.60D-07 CP: 9.99D-01 1.10D+00 7.83D-01 7.43D-01 8.23D-01

CP: 6.40D-01 8.66D-01

E= -1914.20041564766 Delta-E= -0.000000024006 Rises=F Damp=F

DIIS: error= 2.89D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.20041564766 IErMin= 8 ErrMin= 2.89D-06

ErrMax= 2.89D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.86D-09 BMatP= 8.32D-08

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

Coeff-Com: -0.282D-04 0.134D-02-0.224D-02-0.104D-01-0.463D-01-0.498D-01

Coeff-Com: 0.170D+00 0.938D+00

Coeff: -0.282D-04 0.134D-02-0.224D-02-0.104D-01-0.463D-01-0.498D-01

Coeff: 0.170D+00 0.938D+00

Gap= 0.099 Goal= None Shift= 0.000

Gap= 0.055 Goal= None Shift= 0.000

RMSDP=1.26D-07 MaxDP=8.50D-06 DE=-2.40D-08 OVMax= 9.78D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 6.67D-08 CP: 9.99D-01 1.10D+00 7.84D-01 7.43D-01 8.34D-01

CP: 6.53D-01 1.11D+00 1.21D+00

E= -1914.20041565435 Delta-E= -0.000000006690 Rises=F Damp=F

DIIS: error= 2.05D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.20041565435 IErMin= 9 ErrMin= 2.05D-06

ErrMax= 2.05D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.89D-09 BMatP= 8.86D-09

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

Coeff-Com: -0.136D-03 0.299D-02-0.652D-03-0.108D-01-0.699D-01-0.102D+00

Coeff-Com: -0.133D-01 0.551D+00 0.642D+00

Coeff: -0.136D-03 0.299D-02-0.652D-03-0.108D-01-0.699D-01-0.102D+00

Coeff: -0.133D-01 0.551D+00 0.642D+00

Gap= 0.099 Goal= None Shift= 0.000

Gap= 0.055 Goal= None Shift= 0.000

RMSDP=6.22D-08 MaxDP=3.70D-06 DE=-6.69D-09 OVMax= 3.92D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 3.80D-08 CP: 9.99D-01 1.10D+00 7.84D-01 7.44D-01 8.36D-01

CP: 6.70D-01 1.19D+00 1.38D+00 8.64D-01

E= -1914.20041565639 Delta-E= -0.000000002032 Rises=F Damp=F

DIIS: error= 9.16D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.20041565639 IErMin=10 ErrMin= 9.16D-07

ErrMax= 9.16D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.87D-10 BMatP= 3.89D-09

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

Coeff-Com: -0.337D-04 0.568D-03 0.402D-03-0.566D-03-0.992D-02-0.198D-01

Coeff-Com: -0.442D-01-0.407D-01 0.219D+00 0.895D+00

Coeff: -0.337D-04 0.568D-03 0.402D-03-0.566D-03-0.992D-02-0.198D-01

Coeff: -0.442D-01-0.407D-01 0.219D+00 0.895D+00

Gap= 0.099 Goal= None Shift= 0.000

Gap= 0.055 Goal= None Shift= 0.000

RMSDP=2.94D-08 MaxDP=1.47D-06 DE=-2.03D-09 OVMax= 1.32D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.57D-08 CP: 9.99D-01 1.10D+00 7.84D-01 7.44D-01 8.38D-01

CP: 6.73D-01 1.23D+00 1.44D+00 1.08D+00 1.19D+00

E= -1914.20041565706 Delta-E= -0.000000000675 Rises=F Damp=F

DIIS: error= 4.59D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.20041565706 IErMin=11 ErrMin= 4.59D-07

ErrMax= 4.59D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.51D-10 BMatP= 4.87D-10

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

Coeff-Com: 0.110D-04-0.330D-03 0.311D-03 0.185D-02 0.901D-02 0.109D-01

Coeff-Com: -0.181D-01-0.128D+00-0.373D-01 0.393D+00 0.769D+00

Coeff: 0.110D-04-0.330D-03 0.311D-03 0.185D-02 0.901D-02 0.109D-01

Coeff: -0.181D-01-0.128D+00-0.373D-01 0.393D+00 0.769D+00

Gap= 0.099 Goal= None Shift= 0.000

Gap= 0.055 Goal= None Shift= 0.000

RMSDP=1.43D-08 MaxDP=7.43D-07 DE=-6.75D-10 OVMax= 5.03D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 8.70D-09 CP: 9.99D-01 1.10D+00 7.84D-01 7.44D-01 8.38D-01

CP: 6.74D-01 1.24D+00 1.47D+00 1.17D+00 1.37D+00

CP: 1.20D+00

E= -1914.20041565700 Delta-E= 0.000000000058 Rises=F Damp=F

DIIS: error= 2.22D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=11 EnMin= -1914.20041565706 IErMin=12 ErrMin= 2.22D-07

ErrMax= 2.22D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.42D-11 BMatP= 1.51D-10

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

Coeff-Com: 0.155D-04-0.335D-03 0.219D-04 0.107D-02 0.745D-02 0.117D-01

Coeff-Com: 0.480D-02-0.491D-01-0.884D-01-0.810D-01 0.386D+00 0.808D+00

Coeff: 0.155D-04-0.335D-03 0.219D-04 0.107D-02 0.745D-02 0.117D-01

Coeff: 0.480D-02-0.491D-01-0.884D-01-0.810D-01 0.386D+00 0.808D+00

Gap= 0.099 Goal= None Shift= 0.000

Gap= 0.055 Goal= None Shift= 0.000

RMSDP=9.35D-09 MaxDP=4.26D-07 DE= 5.82D-11 OVMax= 3.37D-06

Error on total polarization charges = 0.07940

SCF Done: E(UB3LYP) = -1914.20041566 A.U. after 12 cycles

NFock= 12 Conv=0.93D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7885 S= 0.5191

<L.S>= 0.000000000000E+00

KE= 1.906190583505D+03 PE=-1.514791255941D+04 EE= 5.960778868022D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.34

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7885, after 0.7512

Leave Link 502 at Sun Aug 18 14:00:04 2019, MaxMem= 2013265920 cpu: 2275.8

(Enter /home/kira/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

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

GePol: Maximum number of non-zero 1st derivatives = 186

Leave Link 701 at Sun Aug 18 14:00:22 2019, MaxMem= 2013265920 cpu: 140.7

(Enter /home/kira/g09/l702.exe)

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

Leave Link 702 at Sun Aug 18 14:00:22 2019, MaxMem= 2013265920 cpu: 0.2

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

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

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

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Sun Aug 18 14:01:00 2019, MaxMem= 2013265920 cpu: 308.1

(Enter /home/kira/g09/l716.exe)

Dipole =-3.16444110D-13 3.85469434D-13-1.61626139D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000441772 0.000102522 -0.000147558

2 6 -0.002475917 -0.000864275 0.000578865

3 7 0.000000000 -0.001060429 -0.001421035

4 6 0.002475917 -0.000864275 0.000578865

5 6 0.000441772 0.000102522 -0.000147558

6 6 -0.000391508 0.000264061 -0.000062854

7 6 -0.001099641 0.000658609 -0.000722452

8 7 -0.000438193 0.000000000 0.001322957

9 6 -0.001099641 -0.000658609 -0.000722452

10 6 0.000003722 -0.000217111 0.000335757

11 6 0.000003722 0.000217111 0.000335757

12 6 0.000391508 0.000264061 -0.000062854

13 6 0.001099641 0.000658609 -0.000722452

14 6 -0.000003722 0.000217111 0.000335757

15 6 -0.000003722 -0.000217111 0.000335757

16 6 0.001099641 -0.000658609 -0.000722452

17 7 0.000438193 0.000000000 0.001322957

18 6 0.000391508 -0.000264061 -0.000062854

19 6 -0.002475917 0.000864275 0.000578865

20 6 -0.000441772 -0.000102522 -0.000147558

21 6 0.000441772 -0.000102522 -0.000147558

22 6 0.002475917 0.000864275 0.000578865

23 7 -0.000000000 0.001060429 -0.001421035

24 6 -0.000391508 -0.000264061 -0.000062854

25 6 -0.000925137 -0.000812167 -0.000079469

26 6 0.000449269 0.000275459 0.000348024

27 6 -0.000101108 0.000111826 0.000021179

28 6 0.000106661 0.000089735 0.000019189

29 6 0.000167827 -0.000064930 -0.000037440

30 6 0.000305834 0.000429847 -0.000302426

31 6 -0.000106661 0.000089735 0.000019189

32 6 0.000101108 0.000111826 0.000021179

33 6 -0.000449269 0.000275459 0.000348024

34 6 0.000925137 -0.000812167 -0.000079469

35 6 -0.000305834 0.000429847 -0.000302426

36 6 -0.000167827 -0.000064930 -0.000037440

37 6 -0.000925137 0.000812167 -0.000079469

38 6 0.000305834 -0.000429847 -0.000302426

39 6 0.000167827 0.000064930 -0.000037440

40 6 0.000106661 -0.000089735 0.000019189

41 6 -0.000101108 -0.000111826 0.000021179

42 6 0.000449269 -0.000275459 0.000348024

43 6 0.000925137 0.000812167 -0.000079469

44 6 -0.000305834 -0.000429847 -0.000302426

45 6 -0.000167827 0.000064930 -0.000037440

46 6 -0.000106661 -0.000089735 0.000019189

47 6 0.000101108 -0.000111826 0.000021179

48 6 -0.000449269 -0.000275459 0.000348024

49 1 -0.000096431 0.000155089 0.000063638

50 1 0.000096431 0.000155089 0.000063638

51 1 0.000220308 -0.000180402 -0.000071450

52 1 0.000220308 0.000180402 -0.000071450

53 1 -0.000220308 0.000180402 -0.000071450

54 1 -0.000220308 -0.000180402 -0.000071450

55 1 -0.000096431 -0.000155089 0.000063638

56 1 0.000096431 -0.000155089 0.000063638

57 1 -0.000096221 -0.000073563 0.000075034

58 1 0.000078845 0.000109831 -0.000023039

59 1 0.000039447 0.000041722 0.000003976

60 1 0.000113433 0.000082506 0.000022765

61 1 -0.000083992 -0.000071890 -0.000057941

62 1 -0.000039447 0.000041722 0.000003976

63 1 -0.000078845 0.000109831 -0.000023039

64 1 0.000096221 -0.000073563 0.000075034

65 1 0.000083992 -0.000071890 -0.000057941

66 1 -0.000113433 0.000082506 0.000022765

67 1 -0.000083992 0.000071890 -0.000057941

68 1 0.000113433 -0.000082506 0.000022765

69 1 0.000039447 -0.000041722 0.000003976

70 1 0.000078845 -0.000109831 -0.000023039

71 1 -0.000096221 0.000073563 0.000075034

72 1 0.000083992 0.000071890 -0.000057941

73 1 -0.000113433 -0.000082506 0.000022765

74 1 -0.000039447 -0.000041722 0.000003976

75 1 -0.000078845 -0.000109831 -0.000023039

76 1 0.000096221 0.000073563 0.000075034

77 1 -0.000000000 0.000354356 0.000170482

78 1 -0.000000000 -0.000354356 0.000170482

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

Cartesian Forces: Max 0.002475917 RMS 0.000509411

Leave Link 716 at Sun Aug 18 14:01:00 2019, MaxMem= 2013265920 cpu: 0.2

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

Internal Forces: Max 0.001664964 RMS 0.000298079

Search for a local minimum.

Step number 3 out of a maximum of 452

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

RMS Force = .29808D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3

DE= -4.52D-04 DEPred=-4.47D-04 R= 1.01D+00

TightC=F SS= 1.41D+00 RLast= 1.95D-01 DXNew= 8.4853D-01 5.8485D-01

Trust test= 1.01D+00 RLast= 1.95D-01 DXMaxT set to 5.85D-01

ITU= 1 1 0

Eigenvalues --- 0.00486 0.00861 0.00861 0.00861 0.01579

Eigenvalues --- 0.01654 0.01668 0.01669 0.01671 0.01690

Eigenvalues --- 0.01690 0.01713 0.01713 0.01713 0.01713

Eigenvalues --- 0.01725 0.01733 0.01827 0.01847 0.01857

Eigenvalues --- 0.01870 0.01880 0.01897 0.01906 0.01907

Eigenvalues --- 0.01947 0.02000 0.02007 0.02010 0.02020

Eigenvalues --- 0.02026 0.02026 0.02041 0.02053 0.02060

Eigenvalues --- 0.02075 0.02083 0.02097 0.02099 0.02099

Eigenvalues --- 0.02099 0.02100 0.02127 0.02132 0.02132

Eigenvalues --- 0.02132 0.02141 0.02141 0.02141 0.02141

Eigenvalues --- 0.02161 0.02161 0.02161 0.02165 0.02165

Eigenvalues --- 0.02165 0.02165 0.02171 0.02171 0.02171

Eigenvalues --- 0.02171 0.02173 0.02175 0.02175 0.02175

Eigenvalues --- 0.02176 0.02176 0.02176 0.02176 0.02197

Eigenvalues --- 0.02212 0.02213 0.02225 0.02227 0.02793

Eigenvalues --- 0.15969 0.15987 0.15987 0.15991 0.15991

Eigenvalues --- 0.15993 0.15994 0.15995 0.15995 0.15995

Eigenvalues --- 0.15995 0.15996 0.15996 0.15996 0.15996

Eigenvalues --- 0.15998 0.15998 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16012 0.16034

Eigenvalues --- 0.21998 0.21998 0.21998 0.21999 0.22000

Eigenvalues --- 0.22000 0.22000 0.22000 0.22778 0.22796

Eigenvalues --- 0.22798 0.22811 0.23477 0.23477 0.23477

Eigenvalues --- 0.23536 0.23564 0.24165 0.24676 0.24730

Eigenvalues --- 0.24850 0.24863 0.24879 0.24998 0.24999

Eigenvalues --- 0.24999 0.24999 0.24999 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.26058 0.28694 0.33146 0.33146 0.33146

Eigenvalues --- 0.33297 0.34576 0.34605 0.35400 0.35400

Eigenvalues --- 0.35400 0.35400 0.35400 0.35400 0.35400

Eigenvalues --- 0.35404 0.35405 0.35405 0.35405 0.35427

Eigenvalues --- 0.35452 0.35452 0.35452 0.35456 0.35461

Eigenvalues --- 0.35461 0.35461 0.35516 0.36108 0.36108

Eigenvalues --- 0.36108 0.36144 0.36232 0.36232 0.36232

Eigenvalues --- 0.36278 0.36866 0.36874 0.37378 0.37407

Eigenvalues --- 0.39533 0.39569 0.41983 0.41983 0.41983

Eigenvalues --- 0.42016 0.42170 0.42170 0.42170 0.42173

Eigenvalues --- 0.43271 0.43533 0.43907 0.44393 0.44418

Eigenvalues --- 0.44743 0.45360 0.45482 0.45558 0.45632

Eigenvalues --- 0.45767 0.45853 0.45854 0.45854 0.45854

Eigenvalues --- 0.46150 0.46150 0.46150 0.46184 0.46286

Eigenvalues --- 0.46644 0.46645 0.46645 0.46645 0.46834

Eigenvalues --- 0.46834 0.46834 0.46855 0.47528 0.48576

Eigenvalues --- 0.48632 0.49022 0.49752 0.49864 0.50658

Eigenvalues --- 0.53094 0.53154 0.55773

En-DIIS/RFO-DIIS IScMMF= 0 using points: 3 2

RFO step: Lambda=-9.53299218D-05.

NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=F DC= 4.52D-04 SmlDif= 1.00D-05

RMS Error= 0.1182864329D-02 NUsed= 2 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.06584 -0.06584

Iteration 1 RMS(Cart)= 0.08704775 RMS(Int)= 0.00205718

Iteration 2 RMS(Cart)= 0.00375106 RMS(Int)= 0.00007878

Iteration 3 RMS(Cart)= 0.00000772 RMS(Int)= 0.00007873

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00007873

ITry= 1 IFail=0 DXMaxC= 2.73D-01 DCOld= 1.00D+10 DXMaxT= 5.85D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 3.46D-08 for atom 69.

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

(Linear) (Quad) (Total)

R1 2.69488 0.00030 -0.00036 -0.00361 -0.00394 2.69094

R2 2.59345 0.00075 0.00034 0.00540 0.00585 2.59931

R3 2.03553 0.00019 -0.00007 -0.00015 -0.00022 2.03532

R4 2.58924 0.00093 -0.00018 -0.00079 -0.00106 2.58818

R5 2.67259 -0.00166 0.00066 0.00435 0.00502 2.67761

R6 2.58924 0.00093 -0.00018 -0.00079 -0.00106 2.58818

R7 1.91387 -0.00037 -0.00007 -0.00135 -0.00143 1.91245

R8 2.69488 0.00030 -0.00036 -0.00361 -0.00394 2.69094

R9 2.67259 -0.00166 0.00066 0.00435 0.00502 2.67761

R10 2.03553 0.00019 -0.00007 -0.00015 -0.00022 2.03532

R11 2.66451 -0.00089 0.00022 0.00016 0.00038 2.66489

R12 2.80419 0.00012 -0.00025 -0.00345 -0.00370 2.80049

R13 2.58112 0.00045 0.00009 0.00135 0.00135 2.58247

R14 2.75012 0.00010 -0.00017 -0.00167 -0.00180 2.74831

R15 2.58112 0.00045 0.00009 0.00135 0.00135 2.58247

R16 2.75012 0.00010 -0.00017 -0.00167 -0.00180 2.74831

R17 2.66451 -0.00089 0.00022 0.00016 0.00038 2.66489

R18 2.56026 0.00014 0.00010 0.00124 0.00146 2.56172

R19 2.03723 0.00029 -0.00005 0.00024 0.00018 2.03741

R20 2.03723 0.00029 -0.00005 0.00024 0.00018 2.03741

R21 2.66451 -0.00089 0.00022 0.00016 0.00038 2.66489

R22 2.80419 0.00012 -0.00025 -0.00345 -0.00370 2.80049

R23 2.75012 0.00010 -0.00017 -0.00167 -0.00180 2.74831

R24 2.58112 0.00045 0.00009 0.00135 0.00135 2.58247

R25 2.56026 0.00014 0.00010 0.00124 0.00146 2.56172

R26 2.03723 0.00029 -0.00005 0.00024 0.00018 2.03741

R27 2.75012 0.00010 -0.00017 -0.00167 -0.00180 2.74831

R28 2.03723 0.00029 -0.00005 0.00024 0.00018 2.03741

R29 2.58112 0.00045 0.00009 0.00135 0.00135 2.58247

R30 2.66451 -0.00089 0.00022 0.00016 0.00038 2.66489

R31 2.67259 -0.00166 0.00066 0.00435 0.00502 2.67761

R32 2.80419 0.00012 -0.00025 -0.00345 -0.00370 2.80049

R33 2.69488 0.00030 -0.00036 -0.00361 -0.00394 2.69094

R34 2.58924 0.00093 -0.00018 -0.00079 -0.00106 2.58818

R35 2.59345 0.00075 0.00034 0.00540 0.00585 2.59931

R36 2.03553 0.00019 -0.00007 -0.00015 -0.00022 2.03532

R37 2.69488 0.00030 -0.00036 -0.00361 -0.00394 2.69094

R38 2.03553 0.00019 -0.00007 -0.00015 -0.00022 2.03532

R39 2.58924 0.00093 -0.00018 -0.00079 -0.00106 2.58818

R40 2.67259 -0.00166 0.00066 0.00435 0.00502 2.67761

R41 1.91387 -0.00037 -0.00007 -0.00135 -0.00143 1.91245

R42 2.80419 0.00012 -0.00025 -0.00345 -0.00370 2.80049

R43 2.64791 0.00015 0.00015 0.00188 0.00203 2.64995

R44 2.64792 0.00023 0.00014 0.00200 0.00214 2.65006

R45 2.62898 0.00025 -0.00002 0.00004 0.00002 2.62900

R46 2.04828 0.00001 -0.00006 -0.00060 -0.00066 2.04762

R47 2.63495 -0.00003 -0.00001 -0.00015 -0.00016 2.63479

R48 2.04932 0.00009 -0.00001 0.00012 0.00011 2.04943

R49 2.63545 -0.00007 -0.00001 -0.00016 -0.00017 2.63527

R50 2.04965 0.00006 -0.00000 0.00009 0.00009 2.04974

R51 2.62837 0.00029 -0.00003 0.00012 0.00009 2.62846

R52 2.04932 0.00009 -0.00001 0.00012 0.00012 2.04944

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R55 2.63545 -0.00007 -0.00001 -0.00016 -0.00017 2.63527

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R57 2.62898 0.00025 -0.00002 0.00004 0.00002 2.62900

R58 2.04932 0.00009 -0.00001 0.00012 0.00011 2.04943

R59 2.64791 0.00015 0.00015 0.00188 0.00203 2.64995

R60 2.04828 0.00001 -0.00006 -0.00060 -0.00066 2.04762

R61 2.64792 0.00023 0.00014 0.00200 0.00214 2.65006

R62 2.62837 0.00029 -0.00003 0.00012 0.00009 2.62846

R63 2.04818 0.00001 -0.00006 -0.00058 -0.00064 2.04754

R64 2.04932 0.00009 -0.00001 0.00012 0.00012 2.04944

R65 2.64792 0.00023 0.00014 0.00200 0.00214 2.65006

R66 2.64791 0.00015 0.00015 0.00188 0.00203 2.64995

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R68 2.04818 0.00001 -0.00006 -0.00058 -0.00064 2.04754

R69 2.63545 -0.00007 -0.00001 -0.00016 -0.00017 2.63527

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R73 2.62898 0.00025 -0.00002 0.00004 0.00002 2.62900

R74 2.04932 0.00009 -0.00001 0.00012 0.00011 2.04943

R75 2.04828 0.00001 -0.00006 -0.00060 -0.00066 2.04762

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R77 2.64791 0.00015 0.00015 0.00188 0.00203 2.64995

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A1 1.88237 0.00012 -0.00006 -0.00076 -0.00085 1.88152

A2 2.18325 -0.00004 0.00013 0.00155 0.00168 2.18493

A3 2.21731 -0.00008 -0.00008 -0.00089 -0.00096 2.21635

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A6 2.20807 0.00010 0.00004 -0.00040 -0.00068 2.20740

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A9 2.18036 -0.00002 -0.00004 -0.00017 -0.00026 2.18010

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A18 2.05818 0.00042 0.00003 0.00224 0.00248 2.06066

A19 2.18645 0.00043 -0.00011 -0.00153 -0.00197 2.18448

A20 2.16206 -0.00063 0.00030 0.00183 0.00241 2.16447

A21 1.93462 0.00020 -0.00019 -0.00015 -0.00039 1.93423

A22 1.84188 -0.00037 0.00018 -0.00013 0.00016 1.84204

A23 1.93462 0.00020 -0.00019 -0.00015 -0.00039 1.93423

A24 2.18645 0.00043 -0.00011 -0.00153 -0.00197 2.18448

A25 2.16206 -0.00063 0.00030 0.00183 0.00241 2.16447

A26 1.85643 -0.00001 0.00008 0.00031 0.00037 1.85680

A27 2.19998 0.00000 -0.00000 0.00016 0.00016 2.20014

A28 2.22643 0.00001 -0.00008 -0.00057 -0.00065 2.22578

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A36 2.18645 0.00043 -0.00011 -0.00153 -0.00197 2.18448

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A54 1.88237 0.00012 -0.00006 -0.00076 -0.00085 1.88152

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A70 2.09581 0.00037 -0.00004 0.00068 0.00065 2.09645

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A73 2.08898 -0.00034 0.00002 -0.00123 -0.00122 2.08776

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A78 2.09316 -0.00016 0.00005 0.00000 0.00005 2.09320

A79 2.09503 0.00008 -0.00002 0.00003 0.00000 2.09504

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A106 2.10240 0.00032 0.00003 0.00124 0.00126 2.10367

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A129 2.09710 0.00001 0.00002 0.00017 0.00019 2.09729

A130 2.08802 0.00010 0.00002 0.00079 0.00081 2.08883

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A134 2.09503 0.00008 -0.00002 0.00003 0.00000 2.09504

A135 2.09702 0.00003 0.00001 0.00021 0.00023 2.09725

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D3 -3.10103 -0.00009 0.00112 0.00632 0.00744 -3.09359

D4 0.03255 0.00014 0.00057 0.01406 0.01462 0.04717

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D6 -3.11824 0.00000 0.00040 0.00481 0.00521 -3.11302

D7 3.11824 -0.00000 -0.00040 -0.00481 -0.00521 3.11302

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D9 -0.02957 0.00015 -0.00120 -0.00266 -0.00385 -0.03342

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D11 3.12005 -0.00008 -0.00065 -0.01042 -0.01104 3.10901

D12 -0.03500 -0.00017 0.00018 -0.00701 -0.00683 -0.04183

D13 -3.02780 0.00007 0.00231 0.02757 0.02988 -2.99793

D14 0.11060 0.00008 0.00234 0.02794 0.03028 0.14088

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D16 -3.04052 0.00035 0.00169 0.03716 0.03882 -3.00170

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D19 -3.09857 -0.00007 0.00037 -0.00074 -0.00036 -3.09893

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D28 -0.11060 -0.00008 -0.00234 -0.02794 -0.03028 -0.14088

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D31 3.02877 -0.00035 -0.00116 -0.03270 -0.03384 2.99493

D32 -0.12510 0.00005 -0.00189 -0.01556 -0.01744 -0.14255

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D35 2.09068 0.00036 0.00091 0.06126 0.06217 2.15285

D36 -1.05037 0.00037 0.00098 0.06240 0.06339 -0.98698

D37 -3.11585 0.00007 0.00061 0.01100 0.01156 -3.10429

D38 0.03666 -0.00027 0.00125 -0.00424 -0.00299 0.03366

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D56 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D57 -3.01972 -0.00004 0.00192 0.01593 0.01785 -3.00187

D58 0.10959 0.00035 0.00120 0.03307 0.03424 0.14383

D59 0.12510 -0.00005 0.00189 0.01556 0.01744 0.14255

D60 -3.02877 0.00035 0.00116 0.03270 0.03384 -2.99493

D61 1.05384 -0.00036 -0.00094 -0.06159 -0.06252 0.99132

D62 -2.08829 -0.00037 -0.00101 -0.06273 -0.06374 -2.15203

D63 -2.09068 -0.00036 -0.00091 -0.06126 -0.06217 -2.15285

D64 1.05037 -0.00037 -0.00098 -0.06240 -0.06339 0.98698

D65 -3.12921 0.00018 0.00016 0.01229 0.01244 -3.11677

D66 0.03920 0.00019 0.00043 0.01609 0.01651 0.05571

D67 0.02311 -0.00017 0.00079 -0.00267 -0.00189 0.02123

D68 -3.09166 -0.00016 0.00106 0.00113 0.00219 -3.08947

D69 3.11585 -0.00007 -0.00061 -0.01100 -0.01156 3.10429

D70 -0.03666 0.00027 -0.00125 0.00424 0.00299 -0.03366

D71 0.00000 -0.00000 -0.00000 -0.00000 0.00000 0.00000

D72 -3.11424 0.00001 0.00028 0.00386 0.00414 -3.11010

D73 3.11424 -0.00001 -0.00028 -0.00386 -0.00414 3.11010

D74 -0.00000 0.00000 -0.00000 -0.00000 0.00000 0.00000

D75 -0.02311 0.00017 -0.00079 0.00267 0.00189 -0.02123

D76 3.12921 -0.00018 -0.00016 -0.01229 -0.01244 3.11677

D77 3.09166 0.00016 -0.00106 -0.00113 -0.00219 3.08947

D78 -0.03920 -0.00019 -0.00043 -0.01609 -0.01651 -0.05571

D79 0.03666 -0.00027 0.00125 -0.00424 -0.00299 0.03366

D80 -3.11585 0.00007 0.00061 0.01100 0.01156 -3.10429

D81 3.01972 0.00004 -0.00192 -0.01593 -0.01785 3.00187

D82 -0.12510 0.00005 -0.00189 -0.01556 -0.01744 -0.14255

D83 -0.10959 -0.00035 -0.00120 -0.03307 -0.03424 -0.14383

D84 3.02877 -0.00035 -0.00116 -0.03270 -0.03384 2.99493

D85 3.02780 -0.00007 -0.00231 -0.02757 -0.02988 2.99793

D86 -0.10426 -0.00035 -0.00166 -0.03679 -0.03842 -0.14268

D87 -0.11060 -0.00008 -0.00234 -0.02794 -0.03028 -0.14088

D88 3.04052 -0.00035 -0.00169 -0.03716 -0.03882 3.00170

D89 -1.05037 0.00037 0.00098 0.06240 0.06339 -0.98698

D90 2.09068 0.00036 0.00091 0.06126 0.06217 2.15285

D91 2.08829 0.00037 0.00101 0.06273 0.06374 2.15203

D92 -1.05384 0.00036 0.00094 0.06159 0.06252 -0.99132

D93 3.13182 -0.00014 -0.00017 -0.00934 -0.00948 3.12234

D94 -0.03255 -0.00014 -0.00057 -0.01406 -0.01462 -0.04717

D95 -0.01778 0.00009 -0.00072 -0.00159 -0.00230 -0.02008

D96 3.10103 0.00009 -0.00112 -0.00632 -0.00744 3.09359

D97 -3.12005 0.00008 0.00065 0.01042 0.01104 -3.10901

D98 0.03500 0.00017 -0.00018 0.00701 0.00683 0.04183

D99 0.02957 -0.00015 0.00120 0.00266 0.00385 0.03342

D100 -3.09857 -0.00007 0.00037 -0.00074 -0.00036 -3.09893

D101 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D102 3.11824 -0.00000 -0.00040 -0.00481 -0.00521 3.11302

D103 -3.11824 0.00000 0.00040 0.00481 0.00521 -3.11302

D104 -0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D105 0.01778 -0.00009 0.00072 0.00159 0.00230 0.02008

D106 -3.13182 0.00014 0.00017 0.00934 0.00948 -3.12234

D107 -3.10103 -0.00009 0.00112 0.00632 0.00744 -3.09359

D108 0.03255 0.00014 0.00057 0.01406 0.01462 0.04717

D109 -0.02957 0.00015 -0.00120 -0.00266 -0.00385 -0.03342

D110 3.09857 0.00007 -0.00037 0.00074 0.00036 3.09893

D111 3.12005 -0.00008 -0.00065 -0.01042 -0.01104 3.10901

D112 -0.03500 -0.00017 0.00018 -0.00701 -0.00683 -0.04183

D113 -3.02780 0.00007 0.00231 0.02757 0.02988 -2.99793

D114 0.11060 0.00008 0.00234 0.02794 0.03028 0.14088

D115 0.10426 0.00035 0.00166 0.03679 0.03842 0.14268

D116 -3.04052 0.00035 0.00169 0.03716 0.03882 -3.00170

D117 1.05037 -0.00037 -0.00098 -0.06240 -0.06339 0.98698

D118 -2.09068 -0.00036 -0.00091 -0.06126 -0.06217 -2.15285

D119 -2.08829 -0.00037 -0.00101 -0.06273 -0.06374 -2.15203

D120 1.05384 -0.00036 -0.00094 -0.06159 -0.06252 0.99132

D121 -3.13043 -0.00003 0.00022 0.00148 0.00170 -3.12873

D122 -0.01355 0.00004 -0.00030 -0.00087 -0.00117 -0.01472

D123 0.01063 -0.00003 0.00015 0.00034 0.00048 0.01111

D124 3.12750 0.00004 -0.00037 -0.00201 -0.00238 3.12512

D125 -3.13168 -0.00005 0.00016 -0.00053 -0.00037 -3.13205

D126 -0.01270 0.00001 -0.00039 -0.00332 -0.00371 -0.01641

D127 0.01045 -0.00004 0.00023 0.00061 0.00084 0.01128

D128 3.12943 0.00002 -0.00032 -0.00218 -0.00250 3.12693

D129 -0.02116 0.00007 -0.00036 -0.00089 -0.00125 -0.02241

D130 3.12250 0.00004 -0.00039 -0.00254 -0.00294 3.11956

D131 -3.13792 0.00001 0.00016 0.00149 0.00165 -3.13627

D132 0.00574 -0.00003 0.00013 -0.00016 -0.00003 0.00571

D133 0.01060 -0.00004 0.00019 0.00049 0.00069 0.01129

D134 -3.13113 -0.00004 0.00019 0.00062 0.00081 -3.13032

D135 -3.13307 -0.00000 0.00023 0.00216 0.00238 -3.13069

D136 0.00838 -0.00000 0.00023 0.00228 0.00251 0.01089

D137 0.01053 -0.00004 0.00018 0.00045 0.00064 0.01117

D138 -3.13351 0.00000 0.00022 0.00236 0.00258 -3.13093

D139 -3.13093 -0.00004 0.00019 0.00033 0.00051 -3.13041

D140 0.00822 -0.00000 0.00022 0.00223 0.00246 0.01067

D141 -0.02104 0.00008 -0.00040 -0.00101 -0.00140 -0.02244

D142 -3.13990 0.00002 0.00016 0.00182 0.00198 -3.13792

D143 3.12299 0.00004 -0.00043 -0.00290 -0.00334 3.11966

D144 0.00413 -0.00003 0.00012 -0.00008 0.00004 0.00418

D145 -0.01060 0.00004 -0.00019 -0.00049 -0.00069 -0.01129

D146 3.13307 0.00000 -0.00023 -0.00216 -0.00238 3.13069

D147 3.13113 0.00004 -0.00019 -0.00062 -0.00081 3.13032

D148 -0.00838 0.00000 -0.00023 -0.00228 -0.00251 -0.01089

D149 -0.01053 0.00004 -0.00018 -0.00045 -0.00064 -0.01117

D150 3.13351 -0.00000 -0.00022 -0.00236 -0.00258 3.13093

D151 3.13093 0.00004 -0.00019 -0.00033 -0.00051 3.13041

D152 -0.00822 0.00000 -0.00022 -0.00223 -0.00246 -0.01067

D153 0.02116 -0.00007 0.00036 0.00089 0.00125 0.02241

D154 3.13792 -0.00001 -0.00016 -0.00149 -0.00165 3.13627

D155 -3.12250 -0.00004 0.00039 0.00254 0.00294 -3.11956

D156 -0.00574 0.00003 -0.00013 0.00016 0.00003 -0.00571

D157 3.13043 0.00003 -0.00022 -0.00148 -0.00170 3.12873

D158 -0.01063 0.00003 -0.00015 -0.00034 -0.00048 -0.01111

D159 0.01355 -0.00004 0.00030 0.00087 0.00117 0.01472

D160 -3.12750 -0.00004 0.00037 0.00201 0.00238 -3.12512

D161 3.13168 0.00005 -0.00016 0.00053 0.00037 3.13205

D162 0.01270 -0.00001 0.00039 0.00332 0.00371 0.01641

D163 -0.01045 0.00004 -0.00023 -0.00061 -0.00084 -0.01128

D164 -3.12943 -0.00002 0.00032 0.00218 0.00250 -3.12693

D165 0.02104 -0.00008 0.00040 0.00101 0.00140 0.02244

D166 -3.12299 -0.00004 0.00043 0.00290 0.00334 -3.11966

D167 3.13990 -0.00002 -0.00016 -0.00182 -0.00198 3.13792

D168 -0.00413 0.00003 -0.00012 0.00008 -0.00004 -0.00418

D169 3.13168 0.00005 -0.00016 0.00053 0.00037 3.13205

D170 0.01270 -0.00001 0.00039 0.00332 0.00371 0.01641

D171 -0.01045 0.00004 -0.00023 -0.00061 -0.00084 -0.01128

D172 -3.12943 -0.00002 0.00032 0.00218 0.00250 -3.12693

D173 3.13043 0.00003 -0.00022 -0.00148 -0.00170 3.12873

D174 0.01355 -0.00004 0.00030 0.00087 0.00117 0.01472

D175 -0.01063 0.00003 -0.00015 -0.00034 -0.00048 -0.01111

D176 -3.12750 -0.00004 0.00037 0.00201 0.00238 -3.12512

D177 0.02104 -0.00008 0.00040 0.00101 0.00140 0.02244

D178 -3.12299 -0.00004 0.00043 0.00290 0.00334 -3.11966

D179 3.13990 -0.00002 -0.00016 -0.00182 -0.00198 3.13792

D180 -0.00413 0.00003 -0.00012 0.00008 -0.00004 -0.00418

D181 -0.01053 0.00004 -0.00018 -0.00045 -0.00064 -0.01117

D182 3.13093 0.00004 -0.00019 -0.00033 -0.00051 3.13041

D183 3.13351 -0.00000 -0.00022 -0.00236 -0.00258 3.13093

D184 -0.00822 0.00000 -0.00022 -0.00223 -0.00246 -0.01067

D185 -0.01060 0.00004 -0.00019 -0.00049 -0.00069 -0.01129

D186 3.13307 0.00000 -0.00023 -0.00216 -0.00238 3.13069

D187 3.13113 0.00004 -0.00019 -0.00062 -0.00081 3.13032

D188 -0.00838 0.00000 -0.00023 -0.00228 -0.00251 -0.01089

D189 0.02116 -0.00007 0.00036 0.00089 0.00125 0.02241

D190 3.13792 -0.00001 -0.00016 -0.00149 -0.00165 3.13627

D191 -3.12250 -0.00004 0.00039 0.00254 0.00294 -3.11956

D192 -0.00574 0.00003 -0.00013 0.00016 0.00003 -0.00571

D193 -3.13168 -0.00005 0.00016 -0.00053 -0.00037 -3.13205

D194 -0.01270 0.00001 -0.00039 -0.00332 -0.00371 -0.01641

D195 0.01045 -0.00004 0.00023 0.00061 0.00084 0.01128

D196 3.12943 0.00002 -0.00032 -0.00218 -0.00250 3.12693

D197 -3.13043 -0.00003 0.00022 0.00148 0.00170 -3.12873

D198 -0.01355 0.00004 -0.00030 -0.00087 -0.00117 -0.01472

D199 0.01063 -0.00003 0.00015 0.00034 0.00048 0.01111

D200 3.12750 0.00004 -0.00037 -0.00201 -0.00238 3.12512

D201 -0.02104 0.00008 -0.00040 -0.00101 -0.00140 -0.02244

D202 3.12299 0.00004 -0.00043 -0.00290 -0.00334 3.11966

D203 -3.13990 0.00002 0.00016 0.00182 0.00198 -3.13792

D204 0.00413 -0.00003 0.00012 -0.00008 0.00004 0.00418

D205 0.01053 -0.00004 0.00018 0.00045 0.00064 0.01117

D206 -3.13093 -0.00004 0.00019 0.00033 0.00051 -3.13041

D207 -3.13351 0.00000 0.00022 0.00236 0.00258 -3.13093

D208 0.00822 -0.00000 0.00022 0.00223 0.00246 0.01067

D209 0.01060 -0.00004 0.00019 0.00049 0.00069 0.01129

D210 -3.13307 -0.00000 0.00023 0.00216 0.00238 -3.13069

D211 -3.13113 -0.00004 0.00019 0.00062 0.00081 -3.13032

D212 0.00838 -0.00000 0.00023 0.00228 0.00251 0.01089

D213 -0.02116 0.00007 -0.00036 -0.00089 -0.00125 -0.02241

D214 -3.13792 0.00001 0.00016 0.00149 0.00165 -3.13627

D215 3.12250 0.00004 -0.00039 -0.00254 -0.00294 3.11956

D216 0.00574 -0.00003 0.00013 -0.00016 -0.00003 0.00571

Item Value Threshold Converged?

Maximum Force 0.001665 0.000450 NO

RMS Force 0.000298 0.000300 YES

Maximum Displacement 0.273040 0.001800 NO

RMS Displacement 0.088397 0.001200 NO

Predicted change in Energy=-3.080456D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Aug 18 14:01:01 2019, MaxMem= 2013265920 cpu: 1.3

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

Stoichiometry C44H30N4(1+,2)

Framework group C2V[SGV(H2N2),SGV'(N2),X(C44H28)]

Deg. of freedom 59

Full point group C2V NOp 4

RotChk: IX=0 Diff= 4.97D-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 -0.687747 4.196711 0.388809

2 6 0 -1.123126 2.870187 0.108606

3 7 0 0.000000 2.098263 -0.027577

4 6 0 1.123126 2.870187 0.108606

5 6 0 0.687747 4.196711 0.388809

6 6 0 2.465593 2.431737 -0.006437

7 6 0 2.877963 1.088103 -0.121577

8 7 0 2.063322 -0.000000 0.019667

9 6 0 2.877963 -1.088103 -0.121577

10 6 0 4.244165 -0.677802 -0.404885

11 6 0 4.244165 0.677802 -0.404885

12 6 0 -2.465593 2.431737 -0.006437

13 6 0 -2.877963 1.088103 -0.121577

14 6 0 -4.244165 0.677802 -0.404885

15 6 0 -4.244165 -0.677802 -0.404885

16 6 0 -2.877963 -1.088103 -0.121577

17 7 0 -2.063322 0.000000 0.019667

18 6 0 -2.465593 -2.431737 -0.006437

19 6 0 -1.123126 -2.870187 0.108606

20 6 0 -0.687747 -4.196711 0.388809

21 6 0 0.687747 -4.196711 0.388809

22 6 0 1.123126 -2.870187 0.108606

23 7 0 -0.000000 -2.098263 -0.027577

24 6 0 2.465593 -2.431737 -0.006437

25 6 0 3.509653 3.483446 -0.000271

26 6 0 3.480325 4.521890 -0.942180

27 6 0 4.472688 5.496913 -0.939448

28 6 0 5.486810 5.461693 0.016743

29 6 0 5.514327 4.439106 0.964510

30 6 0 4.540072 3.446491 0.950238

31 6 0 -5.486810 5.461693 0.016743

32 6 0 -4.472688 5.496913 -0.939448

33 6 0 -3.480325 4.521890 -0.942180

34 6 0 -3.509653 3.483446 -0.000271

35 6 0 -4.540072 3.446491 0.950238

36 6 0 -5.514327 4.439106 0.964510

37 6 0 3.509653 -3.483446 -0.000271

38 6 0 4.540072 -3.446491 0.950238

39 6 0 5.514327 -4.439106 0.964510

40 6 0 5.486810 -5.461693 0.016743

41 6 0 4.472688 -5.496913 -0.939448

42 6 0 3.480325 -4.521890 -0.942180

43 6 0 -3.509653 -3.483446 -0.000271

44 6 0 -4.540072 -3.446491 0.950238

45 6 0 -5.514327 -4.439106 0.964510

46 6 0 -5.486810 -5.461693 0.016743

47 6 0 -4.472688 -5.496913 -0.939448

48 6 0 -3.480325 -4.521890 -0.942180

49 1 0 -1.335741 5.033020 0.590579

50 1 0 1.335741 5.033020 0.590579

51 1 0 5.075508 -1.334553 -0.604777

52 1 0 5.075508 1.334553 -0.604777

53 1 0 -5.075508 1.334553 -0.604777

54 1 0 -5.075508 -1.334553 -0.604777

55 1 0 -1.335741 -5.033020 0.590579

56 1 0 1.335741 -5.033020 0.590579

57 1 0 2.694869 4.546210 -1.688207

58 1 0 4.453456 6.284765 -1.684490

59 1 0 6.253583 6.228854 0.023458

60 1 0 6.295840 4.413757 1.716020

61 1 0 4.558796 2.653524 1.688377

62 1 0 -6.253583 6.228854 0.023458

63 1 0 -4.453456 6.284765 -1.684490

64 1 0 -2.694869 4.546210 -1.688207

65 1 0 -4.558796 2.653524 1.688377

66 1 0 -6.295840 4.413757 1.716020

67 1 0 4.558796 -2.653524 1.688377

68 1 0 6.295840 -4.413757 1.716020

69 1 0 6.253583 -6.228854 0.023458

70 1 0 4.453456 -6.284765 -1.684490

71 1 0 2.694869 -4.546210 -1.688207

72 1 0 -4.558796 -2.653524 1.688377

73 1 0 -6.295840 -4.413757 1.716020

74 1 0 -6.253583 -6.228854 0.023458

75 1 0 -4.453456 -6.284765 -1.684490

76 1 0 -2.694869 -4.546210 -1.688207

77 1 0 0.000000 1.100326 -0.195843

78 1 0 -0.000000 -1.100326 -0.195843

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

Rotational constants (GHZ): 0.0591412 0.0584690 0.0302414

Leave Link 202 at Sun Aug 18 14:01:01 2019, MaxMem= 2013265920 cpu: 0.1

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

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

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

There are 261 symmetry adapted cartesian basis functions of A1 symmetry.

There are 240 symmetry adapted cartesian basis functions of A2 symmetry.

There are 249 symmetry adapted cartesian basis functions of B1 symmetry.

There are 252 symmetry adapted cartesian basis functions of B2 symmetry.

There are 248 symmetry adapted basis functions of A1 symmetry.

There are 229 symmetry adapted basis functions of A2 symmetry.

There are 237 symmetry adapted basis functions of B1 symmetry.

There are 240 symmetry adapted basis functions of B2 symmetry.

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

161 alpha electrons 160 beta electrons

nuclear repulsion energy 5368.9961262922 Hartrees.

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

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

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

NAtoms= 78 NActive= 78 NUniq= 21 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=T Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2128229183 Hartrees.

Nuclear repulsion after empirical dispersion term = 5368.7833033739 Hartrees.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 78

GePol: Total number of spheres = 78

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

GePol: Number of points = 5744

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.53D-09

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 274

GePol: Fraction of low-weight points (<1% of avg) = 4.77%

GePol: Cavity surface area = 608.000 Ang\*\*2

GePol: Cavity volume = 625.671 Ang\*\*3

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

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

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PCM non-electrostatic energy = -0.0021997539 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5368.7811036201 Hartrees.

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(Enter /home/kira/g09/l302.exe)

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

NBasis= 954 RedAO= T EigKep= 6.33D-05 NBF= 248 229 237 240

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 248 229 237 240

Precomputing XC quadrature grid using

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

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

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

Leave Link 302 at Sun Aug 18 14:01:02 2019, MaxMem= 2013265920 cpu: 10.1

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

DipDrv: MaxL=1.

Leave Link 303 at Sun Aug 18 14:01:02 2019, MaxMem= 2013265920 cpu: 1.3

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

Initial guess from the checkpoint file: "TPPcation.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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(B2) (B2) (B2) (B2)

The electronic state of the initial guess is 2-A1.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7885 S= 0.5191

Generating alternative initial guess.

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -1914.09084687267

Leave Link 401 at Sun Aug 18 14:01:08 2019, MaxMem= 2013265920 cpu: 47.2

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3049894 IEndB= 3049894 NGot= 2013265920 MDV= 2011237673

LenX= 2011237673 LenY= 2010232667

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

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

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

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

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

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 98980608.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.00D-15 for 5713.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.33D-15 for 4975 4828.

Iteration 1 A^-1\*A deviation from unit magnitude is 4.44D-15 for 5724.

Iteration 1 A^-1\*A deviation from orthogonality is 4.21D-13 for 5437 5422.

E= -1914.13694724260

DIIS: error= 9.69D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.13694724260 IErMin= 1 ErrMin= 9.69D-03

ErrMax= 9.69D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.17D-01 BMatP= 1.17D-01

IDIUse=3 WtCom= 9.03D-01 WtEn= 9.69D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.502 Goal= None Shift= 0.000

Gap= 0.515 Goal= None Shift= 0.000

GapD= 0.502 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=2.40D-04 MaxDP=7.17D-03 OVMax= 4.34D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.40D-04 CP: 9.98D-01

E= -1914.19975927087 Delta-E= -0.062812028271 Rises=F Damp=F

DIIS: error= 1.33D-03 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.19975927087 IErMin= 2 ErrMin= 1.33D-03

ErrMax= 1.33D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.73D-03 BMatP= 1.17D-01

IDIUse=3 WtCom= 9.87D-01 WtEn= 1.33D-02

Coeff-Com: -0.711D-01 0.107D+01

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

Coeff: -0.702D-01 0.107D+01

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=4.44D-05 MaxDP=9.66D-04 DE=-6.28D-02 OVMax= 6.82D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.99D-05 CP: 9.98D-01 1.08D+00

E= -1914.20080081262 Delta-E= -0.001041541748 Rises=F Damp=F

DIIS: error= 2.74D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.20080081262 IErMin= 3 ErrMin= 2.74D-04

ErrMax= 2.74D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.14D-04 BMatP= 1.73D-03

IDIUse=3 WtCom= 9.97D-01 WtEn= 2.74D-03

Coeff-Com: -0.271D-01 0.319D+00 0.708D+00

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

Coeff: -0.270D-01 0.318D+00 0.709D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.057 Goal= None Shift= 0.000

RMSDP=1.46D-05 MaxDP=6.37D-04 DE=-1.04D-03 OVMax= 3.28D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.26D-05 CP: 9.98D-01 1.10D+00 8.38D-01

E= -1914.20085647480 Delta-E= -0.000055662186 Rises=F Damp=F

DIIS: error= 1.96D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.20085647480 IErMin= 4 ErrMin= 1.96D-04

ErrMax= 1.96D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.25D-04 BMatP= 3.14D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.96D-03

Coeff-Com: -0.838D-02 0.770D-01 0.393D+00 0.538D+00

Coeff-En: 0.000D+00 0.000D+00 0.219D+00 0.781D+00

Coeff: -0.837D-02 0.769D-01 0.393D+00 0.539D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=6.75D-06 MaxDP=4.16D-04 DE=-5.57D-05 OVMax= 1.97D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.76D-06 CP: 9.98D-01 1.10D+00 8.89D-01 6.65D-01

E= -1914.20088441498 Delta-E= -0.000027940182 Rises=F Damp=F

DIIS: error= 8.08D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.20088441498 IErMin= 5 ErrMin= 8.08D-05

ErrMax= 8.08D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.34D-05 BMatP= 1.25D-04

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

Coeff-Com: -0.595D-03-0.695D-02 0.102D+00 0.281D+00 0.625D+00

Coeff: -0.595D-03-0.695D-02 0.102D+00 0.281D+00 0.625D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=3.01D-06 MaxDP=2.39D-04 DE=-2.79D-05 OVMax= 8.29D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.07D-06 CP: 9.98D-01 1.10D+00 9.01D-01 7.53D-01 6.24D-01

E= -1914.20088686637 Delta-E= -0.000002451390 Rises=F Damp=F

DIIS: error= 3.82D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.20088686637 IErMin= 6 ErrMin= 3.82D-05

ErrMax= 3.82D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.82D-06 BMatP= 1.34D-05

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

Coeff-Com: 0.856D-03-0.163D-01 0.662D-02 0.101D+00 0.407D+00 0.501D+00

Coeff: 0.856D-03-0.163D-01 0.662D-02 0.101D+00 0.407D+00 0.501D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=1.29D-06 MaxDP=1.06D-04 DE=-2.45D-06 OVMax= 5.78D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 6.04D-07 CP: 9.98D-01 1.10D+00 9.10D-01 7.48D-01 7.49D-01

CP: 5.68D-01

E= -1914.20088786203 Delta-E= -0.000000995655 Rises=F Damp=F

DIIS: error= 9.99D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.20088786203 IErMin= 7 ErrMin= 9.99D-06

ErrMax= 9.99D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.36D-07 BMatP= 3.82D-06

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

Coeff-Com: 0.381D-03-0.637D-02-0.185D-02 0.298D-01 0.140D+00 0.220D+00

Coeff-Com: 0.619D+00

Coeff: 0.381D-03-0.637D-02-0.185D-02 0.298D-01 0.140D+00 0.220D+00

Coeff: 0.619D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=3.04D-07 MaxDP=2.46D-05 DE=-9.96D-07 OVMax= 1.06D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.47D-07 CP: 9.98D-01 1.10D+00 9.10D-01 7.57D-01 7.45D-01

CP: 6.22D-01 1.14D+00

E= -1914.20088792759 Delta-E= -0.000000065561 Rises=F Damp=F

DIIS: error= 6.81D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.20088792759 IErMin= 8 ErrMin= 6.81D-06

ErrMax= 6.81D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.17D-08 BMatP= 1.36D-07

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

Coeff-Com: -0.246D-03 0.526D-02-0.480D-02-0.383D-01-0.146D+00-0.137D+00

Coeff-Com: 0.364D+00 0.957D+00

Coeff: -0.246D-03 0.526D-02-0.480D-02-0.383D-01-0.146D+00-0.137D+00

Coeff: 0.364D+00 0.957D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=3.26D-07 MaxDP=2.83D-05 DE=-6.56D-08 OVMax= 1.59D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.30D-07 CP: 9.98D-01 1.10D+00 9.11D-01 7.58D-01 7.61D-01

CP: 6.77D-01 1.56D+00 1.18D+00

E= -1914.20088798286 Delta-E= -0.000000055269 Rises=F Damp=F

DIIS: error= 2.90D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.20088798286 IErMin= 9 ErrMin= 2.90D-06

ErrMax= 2.90D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.10D-08 BMatP= 5.17D-08

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

Coeff-Com: -0.179D-03 0.346D-02-0.144D-02-0.218D-01-0.904D-01-0.101D+00

Coeff-Com: 0.289D-01 0.400D+00 0.782D+00

Coeff: -0.179D-03 0.346D-02-0.144D-02-0.218D-01-0.904D-01-0.101D+00

Coeff: 0.289D-01 0.400D+00 0.782D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=1.41D-07 MaxDP=1.01D-05 DE=-5.53D-08 OVMax= 5.49D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 7.05D-08 CP: 9.98D-01 1.10D+00 9.11D-01 7.59D-01 7.63D-01

CP: 7.07D-01 1.71D+00 1.37D+00 1.29D+00

E= -1914.20088799362 Delta-E= -0.000000010764 Rises=F Damp=F

DIIS: error= 1.63D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.20088799362 IErMin=10 ErrMin= 1.63D-06

ErrMax= 1.63D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.08D-09 BMatP= 1.10D-08

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

Coeff-Com: 0.172D-04-0.593D-03 0.161D-02 0.632D-02 0.186D-01 0.102D-01

Coeff-Com: -0.149D+00-0.210D+00 0.447D+00 0.877D+00

Coeff: 0.172D-04-0.593D-03 0.161D-02 0.632D-02 0.186D-01 0.102D-01

Coeff: -0.149D+00-0.210D+00 0.447D+00 0.877D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=9.33D-08 MaxDP=6.00D-06 DE=-1.08D-08 OVMax= 3.54D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 3.74D-08 CP: 9.98D-01 1.10D+00 9.11D-01 7.60D-01 7.65D-01

CP: 7.13D-01 1.79D+00 1.52D+00 1.71D+00 1.09D+00

E= -1914.20088799747 Delta-E= -0.000000003844 Rises=F Damp=F

DIIS: error= 9.20D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.20088799747 IErMin=11 ErrMin= 9.20D-07

ErrMax= 9.20D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.13D-10 BMatP= 4.08D-09

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

Coeff-Com: 0.266D-04-0.608D-03 0.718D-03 0.475D-02 0.171D-01 0.154D-01

Coeff-Com: -0.592D-01-0.120D+00 0.708D-01 0.316D+00 0.755D+00

Coeff: 0.266D-04-0.608D-03 0.718D-03 0.475D-02 0.171D-01 0.154D-01

Coeff: -0.592D-01-0.120D+00 0.708D-01 0.316D+00 0.755D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=2.70D-08 MaxDP=1.23D-06 DE=-3.84D-09 OVMax= 9.43D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.76D-08 CP: 9.98D-01 1.10D+00 9.11D-01 7.60D-01 7.65D-01

CP: 7.15D-01 1.80D+00 1.54D+00 1.81D+00 1.27D+00

CP: 1.14D+00

E= -1914.20088799791 Delta-E= -0.000000000447 Rises=F Damp=F

DIIS: error= 6.34D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.20088799791 IErMin=12 ErrMin= 6.34D-07

ErrMax= 6.34D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.32D-10 BMatP= 5.13D-10

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

Coeff-Com: 0.772D-05-0.982D-04-0.269D-03 0.127D-03 0.224D-02 0.462D-02

Coeff-Com: 0.259D-01 0.162D-01-0.132D+00-0.171D+00 0.424D+00 0.831D+00

Coeff: 0.772D-05-0.982D-04-0.269D-03 0.127D-03 0.224D-02 0.462D-02

Coeff: 0.259D-01 0.162D-01-0.132D+00-0.171D+00 0.424D+00 0.831D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=1.98D-08 MaxDP=8.87D-07 DE=-4.47D-10 OVMax= 9.39D-06

Cycle 13 Pass 1 IDiag 1:

RMSU= 8.85D-09 CP: 9.98D-01 1.10D+00 9.11D-01 7.60D-01 7.65D-01

CP: 7.15D-01 1.80D+00 1.56D+00 1.88D+00 1.37D+00

CP: 1.48D+00 1.17D+00

E= -1914.20088799815 Delta-E= -0.000000000235 Rises=F Damp=F

DIIS: error= 2.68D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1914.20088799815 IErMin=13 ErrMin= 2.68D-07

ErrMax= 2.68D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.30D-11 BMatP= 2.32D-10

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

Coeff-Com: -0.332D-05 0.115D-03-0.325D-03-0.120D-02-0.341D-02-0.194D-02

Coeff-Com: 0.289D-01 0.382D-01-0.790D-01-0.165D+00-0.131D-01 0.369D+00

Coeff-Com: 0.828D+00

Coeff: -0.332D-05 0.115D-03-0.325D-03-0.120D-02-0.341D-02-0.194D-02

Coeff: 0.289D-01 0.382D-01-0.790D-01-0.165D+00-0.131D-01 0.369D+00

Coeff: 0.828D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=9.90D-09 MaxDP=4.17D-07 DE=-2.35D-10 OVMax= 4.30D-06

Error on total polarization charges = 0.07916

SCF Done: E(UB3LYP) = -1914.20088800 A.U. after 13 cycles

NFock= 13 Conv=0.99D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7876 S= 0.5186

<L.S>= 0.000000000000E+00

KE= 1.906182809481D+03 PE=-1.515209018184D+04 EE= 5.962925380745D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.38

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7876, after 0.7512

Leave Link 502 at Sun Aug 18 14:06:17 2019, MaxMem= 2013265920 cpu: 2450.6

(Enter /home/kira/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

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

GePol: Maximum number of non-zero 1st derivatives = 186

Leave Link 701 at Sun Aug 18 14:06:34 2019, MaxMem= 2013265920 cpu: 141.1

(Enter /home/kira/g09/l702.exe)

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

Leave Link 702 at Sun Aug 18 14:06:34 2019, MaxMem= 2013265920 cpu: 0.2

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

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

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

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Sun Aug 18 14:07:13 2019, MaxMem= 2013265920 cpu: 311.9

(Enter /home/kira/g09/l716.exe)

Dipole = 5.23770625D-13 1.40332190D-12-2.05437430D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.002127885 0.000902709 0.000224597

2 6 -0.004430208 -0.001460282 0.000364967

3 7 0.000000000 -0.001498240 -0.001230334

4 6 0.004430208 -0.001460282 0.000364967

5 6 -0.002127885 0.000902709 0.000224597

6 6 -0.001503650 0.000899241 -0.000027274

7 6 -0.001496326 -0.000220914 0.000241757

8 7 -0.000102457 0.000000000 -0.000224049

9 6 -0.001496326 0.000220914 0.000241757

10 6 0.000392638 0.000298733 -0.000181269

11 6 0.000392638 -0.000298733 -0.000181269

12 6 0.001503650 0.000899241 -0.000027274

13 6 0.001496326 -0.000220914 0.000241757

14 6 -0.000392638 -0.000298733 -0.000181269

15 6 -0.000392638 0.000298733 -0.000181269

16 6 0.001496326 0.000220914 0.000241757

17 7 0.000102457 -0.000000000 -0.000224049

18 6 0.001503650 -0.000899241 -0.000027274

19 6 -0.004430208 0.001460282 0.000364967

20 6 0.002127885 -0.000902709 0.000224597

21 6 -0.002127885 -0.000902709 0.000224597

22 6 0.004430208 0.001460282 0.000364967

23 7 -0.000000000 0.001498240 -0.001230334

24 6 -0.001503650 -0.000899241 -0.000027274

25 6 -0.000807153 -0.000864897 -0.000014275

26 6 0.000902653 0.000291065 0.000399106

27 6 -0.000375340 -0.000004162 -0.000178646

28 6 0.000104214 0.000099470 0.000003734

29 6 -0.000013516 -0.000362221 0.000174895

30 6 0.000297271 0.000993728 -0.000342638

31 6 -0.000104214 0.000099470 0.000003734

32 6 0.000375340 -0.000004162 -0.000178646

33 6 -0.000902653 0.000291065 0.000399106

34 6 0.000807153 -0.000864897 -0.000014275

35 6 -0.000297271 0.000993728 -0.000342638

36 6 0.000013516 -0.000362221 0.000174895

37 6 -0.000807153 0.000864897 -0.000014275

38 6 0.000297271 -0.000993728 -0.000342638

39 6 -0.000013516 0.000362221 0.000174895

40 6 0.000104214 -0.000099470 0.000003734

41 6 -0.000375340 0.000004162 -0.000178646

42 6 0.000902653 -0.000291065 0.000399106

43 6 0.000807153 0.000864897 -0.000014275

44 6 -0.000297271 -0.000993728 -0.000342638

45 6 0.000013516 0.000362221 0.000174895

46 6 -0.000104214 -0.000099470 0.000003734

47 6 0.000375340 0.000004162 -0.000178646

48 6 -0.000902653 -0.000291065 0.000399106

49 1 -0.000110087 0.000139471 0.000078841

50 1 0.000110087 0.000139471 0.000078841

51 1 0.000156406 -0.000054080 -0.000140516

52 1 0.000156406 0.000054080 -0.000140516

53 1 -0.000156406 0.000054080 -0.000140516

54 1 -0.000156406 -0.000054080 -0.000140516

55 1 -0.000110087 -0.000139471 0.000078841

56 1 0.000110087 -0.000139471 0.000078841

57 1 -0.000047337 -0.000014452 -0.000190875

58 1 -0.000061363 0.000083874 0.000032099

59 1 0.000012024 0.000010755 -0.000003940

60 1 0.000090392 -0.000063830 -0.000033803

61 1 -0.000032581 -0.000016961 0.000160797

62 1 -0.000012024 0.000010755 -0.000003940

63 1 0.000061363 0.000083874 0.000032099

64 1 0.000047337 -0.000014452 -0.000190875

65 1 0.000032581 -0.000016961 0.000160797

66 1 -0.000090392 -0.000063830 -0.000033803

67 1 -0.000032581 0.000016961 0.000160797

68 1 0.000090392 0.000063830 -0.000033803

69 1 0.000012024 -0.000010755 -0.000003940

70 1 -0.000061363 -0.000083874 0.000032099

71 1 -0.000047337 0.000014452 -0.000190875

72 1 0.000032581 0.000016961 0.000160797

73 1 -0.000090392 0.000063830 -0.000033803

74 1 -0.000012024 -0.000010755 -0.000003940

75 1 0.000061363 -0.000083874 0.000032099

76 1 0.000047337 0.000014452 -0.000190875

77 1 0.000000000 0.000343978 0.000319273

78 1 -0.000000000 -0.000343978 0.000319273

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

Cartesian Forces: Max 0.004430208 RMS 0.000818399

Leave Link 716 at Sun Aug 18 14:07:14 2019, MaxMem= 2013265920 cpu: 0.2

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

Internal Forces: Max 0.002595720 RMS 0.000386605

Search for a local minimum.

Step number 4 out of a maximum of 452

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

RMS Force = .38660D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 2 3 4

DE= -4.72D-04 DEPred=-3.08D-04 R= 1.53D+00

TightC=F SS= 1.41D+00 RLast= 3.16D-01 DXNew= 9.8360D-01 9.4850D-01

Trust test= 1.53D+00 RLast= 3.16D-01 DXMaxT set to 9.49D-01

ITU= 1 1 1 0

Eigenvalues --- 0.00199 0.00861 0.00861 0.00861 0.01532

Eigenvalues --- 0.01653 0.01669 0.01670 0.01681 0.01688

Eigenvalues --- 0.01691 0.01712 0.01712 0.01712 0.01715

Eigenvalues --- 0.01733 0.01733 0.01828 0.01857 0.01857

Eigenvalues --- 0.01870 0.01903 0.01907 0.01907 0.01908

Eigenvalues --- 0.01948 0.02003 0.02007 0.02011 0.02020

Eigenvalues --- 0.02026 0.02027 0.02041 0.02056 0.02064

Eigenvalues --- 0.02078 0.02087 0.02099 0.02099 0.02099

Eigenvalues --- 0.02099 0.02117 0.02132 0.02132 0.02132

Eigenvalues --- 0.02141 0.02141 0.02141 0.02141 0.02161

Eigenvalues --- 0.02161 0.02161 0.02162 0.02165 0.02165

Eigenvalues --- 0.02165 0.02165 0.02171 0.02171 0.02171

Eigenvalues --- 0.02171 0.02175 0.02175 0.02175 0.02176

Eigenvalues --- 0.02176 0.02176 0.02176 0.02177 0.02212

Eigenvalues --- 0.02214 0.02225 0.02228 0.02452 0.03199

Eigenvalues --- 0.15981 0.15983 0.15983 0.15987 0.15987

Eigenvalues --- 0.15991 0.15993 0.15994 0.15994 0.15994

Eigenvalues --- 0.15994 0.15995 0.15995 0.15995 0.15995

Eigenvalues --- 0.15999 0.15999 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16010 0.16144

Eigenvalues --- 0.21998 0.21998 0.21998 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22008 0.22769 0.22795

Eigenvalues --- 0.22797 0.22807 0.23476 0.23476 0.23476

Eigenvalues --- 0.23533 0.23542 0.24135 0.24352 0.24718

Eigenvalues --- 0.24808 0.24815 0.24928 0.24999 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25149

Eigenvalues --- 0.26050 0.28148 0.33146 0.33146 0.33146

Eigenvalues --- 0.33430 0.34577 0.34606 0.35400 0.35400

Eigenvalues --- 0.35400 0.35400 0.35400 0.35400 0.35400

Eigenvalues --- 0.35404 0.35405 0.35405 0.35405 0.35424

Eigenvalues --- 0.35452 0.35452 0.35452 0.35457 0.35461

Eigenvalues --- 0.35461 0.35461 0.35531 0.36108 0.36108

Eigenvalues --- 0.36108 0.36147 0.36232 0.36232 0.36232

Eigenvalues --- 0.36279 0.36872 0.37058 0.37377 0.37404

Eigenvalues --- 0.39532 0.39924 0.41988 0.41988 0.41988

Eigenvalues --- 0.42160 0.42168 0.42168 0.42168 0.42174

Eigenvalues --- 0.43258 0.43519 0.44387 0.44415 0.44711

Eigenvalues --- 0.45339 0.45353 0.45484 0.45551 0.45632

Eigenvalues --- 0.45829 0.45855 0.45855 0.45855 0.45861

Eigenvalues --- 0.46150 0.46150 0.46150 0.46278 0.46394

Eigenvalues --- 0.46645 0.46645 0.46645 0.46645 0.46834

Eigenvalues --- 0.46834 0.46834 0.46949 0.47522 0.48572

Eigenvalues --- 0.48628 0.49750 0.49861 0.50652 0.51658

Eigenvalues --- 0.53087 0.54413 0.63774

En-DIIS/RFO-DIIS IScMMF= 0 using points: 4 3 2

RFO step: Lambda=-1.27023217D-04.

NNeg= 0 NP= 3 Switch= 2.50D-03 Rises=F DC= 4.52D-04 SmlDif= 1.00D-05

RMS Error= 0.1407251105D-02 NUsed= 3 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.47083 -0.01677 -0.45405

Iteration 1 RMS(Cart)= 0.14300317 RMS(Int)= 0.00480819

Iteration 2 RMS(Cart)= 0.01063207 RMS(Int)= 0.00047786

Iteration 3 RMS(Cart)= 0.00006495 RMS(Int)= 0.00047754

Iteration 4 RMS(Cart)= 0.00000005 RMS(Int)= 0.00047754

ITry= 1 IFail=0 DXMaxC= 5.60D-01 DCOld= 1.00D+10 DXMaxT= 9.49D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 3.20D-08 for atom 62.

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

(Linear) (Quad) (Total)

R1 2.69094 0.00132 -0.00435 0.00105 -0.00310 2.68784

R2 2.59931 -0.00108 0.00513 0.00064 0.00643 2.60573

R3 2.03532 0.00019 -0.00055 0.00044 -0.00012 2.03520

R4 2.58818 0.00124 -0.00177 0.00123 -0.00108 2.58710

R5 2.67761 -0.00260 0.00693 -0.00225 0.00468 2.68228

R6 2.58818 0.00124 -0.00177 0.00123 -0.00108 2.58710

R7 1.91245 -0.00039 -0.00117 -0.00138 -0.00255 1.90990

R8 2.69094 0.00132 -0.00435 0.00105 -0.00310 2.68784

R9 2.67761 -0.00260 0.00693 -0.00225 0.00468 2.68228

R10 2.03532 0.00019 -0.00055 0.00044 -0.00012 2.03520

R11 2.66489 -0.00022 0.00169 -0.00021 0.00148 2.66637

R12 2.80049 0.00016 -0.00345 -0.00305 -0.00650 2.79399

R13 2.58247 0.00006 0.00125 -0.00013 0.00056 2.58304

R14 2.74831 0.00052 -0.00200 0.00057 -0.00123 2.74708

R15 2.58247 0.00006 0.00125 -0.00013 0.00056 2.58304

R16 2.74831 0.00052 -0.00200 0.00057 -0.00123 2.74708

R17 2.66489 -0.00022 0.00169 -0.00021 0.00148 2.66637

R18 2.56172 -0.00046 0.00138 -0.00018 0.00192 2.56363

R19 2.03741 0.00018 -0.00028 0.00054 0.00026 2.03767

R20 2.03741 0.00018 -0.00028 0.00054 0.00026 2.03767

R21 2.66489 -0.00022 0.00169 -0.00021 0.00148 2.66637

R22 2.80049 0.00016 -0.00345 -0.00305 -0.00650 2.79399

R23 2.74831 0.00052 -0.00200 0.00057 -0.00123 2.74708

R24 2.58247 0.00006 0.00125 -0.00013 0.00056 2.58304

R25 2.56172 -0.00046 0.00138 -0.00018 0.00192 2.56363

R26 2.03741 0.00018 -0.00028 0.00054 0.00026 2.03767

R27 2.74831 0.00052 -0.00200 0.00057 -0.00123 2.74708

R28 2.03741 0.00018 -0.00028 0.00054 0.00026 2.03767

R29 2.58247 0.00006 0.00125 -0.00013 0.00056 2.58304

R30 2.66489 -0.00022 0.00169 -0.00021 0.00148 2.66637

R31 2.67761 -0.00260 0.00693 -0.00225 0.00468 2.68228

R32 2.80049 0.00016 -0.00345 -0.00305 -0.00650 2.79399

R33 2.69094 0.00132 -0.00435 0.00105 -0.00310 2.68784

R34 2.58818 0.00124 -0.00177 0.00123 -0.00108 2.58710

R35 2.59931 -0.00108 0.00513 0.00064 0.00643 2.60573

R36 2.03532 0.00019 -0.00055 0.00044 -0.00012 2.03520

R37 2.69094 0.00132 -0.00435 0.00105 -0.00310 2.68784

R38 2.03532 0.00019 -0.00055 0.00044 -0.00012 2.03520

R39 2.58818 0.00124 -0.00177 0.00123 -0.00108 2.58710

R40 2.67761 -0.00260 0.00693 -0.00225 0.00468 2.68228

R41 1.91245 -0.00039 -0.00117 -0.00138 -0.00255 1.90990

R42 2.80049 0.00016 -0.00345 -0.00305 -0.00650 2.79399

R43 2.64995 0.00022 0.00200 0.00155 0.00356 2.65351

R44 2.65006 0.00022 0.00200 0.00157 0.00358 2.65364

R45 2.62900 -0.00018 -0.00015 -0.00087 -0.00103 2.62798

R46 2.04762 0.00017 -0.00073 0.00022 -0.00051 2.04710

R47 2.63479 0.00007 -0.00017 0.00022 0.00005 2.63483

R48 2.04943 0.00004 0.00000 0.00007 0.00007 2.04950

R49 2.63527 0.00007 -0.00014 0.00024 0.00010 2.63537

R50 2.04974 0.00002 0.00002 0.00002 0.00004 2.04978

R51 2.62846 -0.00017 -0.00013 -0.00084 -0.00097 2.62749

R52 2.04944 0.00004 -0.00000 0.00008 0.00008 2.04952

R53 2.04754 0.00012 -0.00070 0.00008 -0.00062 2.04692

R54 2.63479 0.00007 -0.00017 0.00022 0.00005 2.63483

R55 2.63527 0.00007 -0.00014 0.00024 0.00010 2.63537

R56 2.04974 0.00002 0.00002 0.00002 0.00004 2.04978

R57 2.62900 -0.00018 -0.00015 -0.00087 -0.00103 2.62798

R58 2.04943 0.00004 0.00000 0.00007 0.00007 2.04950

R59 2.64995 0.00022 0.00200 0.00155 0.00356 2.65351

R60 2.04762 0.00017 -0.00073 0.00022 -0.00051 2.04710

R61 2.65006 0.00022 0.00200 0.00157 0.00358 2.65364

R62 2.62846 -0.00017 -0.00013 -0.00084 -0.00097 2.62749

R63 2.04754 0.00012 -0.00070 0.00008 -0.00062 2.04692

R64 2.04944 0.00004 -0.00000 0.00008 0.00008 2.04952

R65 2.65006 0.00022 0.00200 0.00157 0.00358 2.65364

R66 2.64995 0.00022 0.00200 0.00155 0.00356 2.65351

R67 2.62846 -0.00017 -0.00013 -0.00084 -0.00097 2.62749

R68 2.04754 0.00012 -0.00070 0.00008 -0.00062 2.04692

R69 2.63527 0.00007 -0.00014 0.00024 0.00010 2.63537

R70 2.04944 0.00004 -0.00000 0.00008 0.00008 2.04952

R71 2.63479 0.00007 -0.00017 0.00022 0.00005 2.63483

R72 2.04974 0.00002 0.00002 0.00002 0.00004 2.04978

R73 2.62900 -0.00018 -0.00015 -0.00087 -0.00103 2.62798

R74 2.04943 0.00004 0.00000 0.00007 0.00007 2.04950

R75 2.04762 0.00017 -0.00073 0.00022 -0.00051 2.04710

R76 2.65006 0.00022 0.00200 0.00157 0.00358 2.65364

R77 2.64995 0.00022 0.00200 0.00155 0.00356 2.65351

R78 2.62846 -0.00017 -0.00013 -0.00084 -0.00097 2.62749

R79 2.04754 0.00012 -0.00070 0.00008 -0.00062 2.04692

R80 2.63527 0.00007 -0.00014 0.00024 0.00010 2.63537

R81 2.04944 0.00004 -0.00000 0.00008 0.00008 2.04952

R82 2.63479 0.00007 -0.00017 0.00022 0.00005 2.63483

R83 2.04974 0.00002 0.00002 0.00002 0.00004 2.04978

R84 2.62900 -0.00018 -0.00015 -0.00087 -0.00103 2.62798

R85 2.04943 0.00004 0.00000 0.00007 0.00007 2.04950

R86 2.04762 0.00017 -0.00073 0.00022 -0.00051 2.04710

A1 1.88152 0.00043 -0.00080 0.00009 -0.00091 1.88061

A2 2.18493 -0.00021 0.00166 0.00069 0.00243 2.18737

A3 2.21635 -0.00021 -0.00097 -0.00077 -0.00166 2.21469

A4 1.86908 -0.00039 0.00024 -0.00011 -0.00001 1.86906

A5 2.20671 0.00050 -0.00017 0.00363 0.00530 2.21201

A6 2.20740 -0.00011 -0.00007 -0.00351 -0.00539 2.20200

A7 1.92294 -0.00008 0.00086 -0.00018 0.00111 1.92406

A8 2.18010 0.00004 -0.00036 0.00012 -0.00054 2.17956

A9 2.18010 0.00004 -0.00036 0.00012 -0.00054 2.17956

A10 1.86908 -0.00039 0.00024 -0.00011 -0.00001 1.86906

A11 2.20740 -0.00011 -0.00007 -0.00351 -0.00539 2.20200

A12 2.20671 0.00050 -0.00017 0.00363 0.00530 2.21201

A13 1.88152 0.00043 -0.00080 0.00009 -0.00091 1.88061

A14 2.21635 -0.00021 -0.00097 -0.00077 -0.00166 2.21469

A15 2.18493 -0.00021 0.00166 0.00069 0.00243 2.18737

A16 2.18770 -0.00069 -0.00211 -0.00697 -0.01161 2.17609

A17 2.03482 0.00016 0.00073 0.00239 0.00438 2.03920

A18 2.06066 0.00053 0.00138 0.00459 0.00723 2.06789

A19 2.18448 0.00049 -0.00172 -0.00254 -0.00603 2.17844

A20 2.16447 -0.00068 0.00322 0.00094 0.00605 2.17051

A21 1.93423 0.00019 -0.00150 0.00155 -0.00019 1.93405

A22 1.84204 -0.00031 0.00133 -0.00225 -0.00044 1.84160

A23 1.93423 0.00019 -0.00150 0.00155 -0.00019 1.93405

A24 2.18448 0.00049 -0.00172 -0.00254 -0.00603 2.17844

A25 2.16447 -0.00068 0.00322 0.00094 0.00605 2.17051

A26 1.85680 -0.00004 0.00072 -0.00073 -0.00019 1.85661

A27 2.20014 0.00009 0.00006 0.00105 0.00119 2.20133

A28 2.22578 -0.00004 -0.00088 -0.00029 -0.00109 2.22469

A29 1.85680 -0.00004 0.00072 -0.00073 -0.00019 1.85661

A30 2.20014 0.00009 0.00006 0.00105 0.00119 2.20133

A31 2.22578 -0.00004 -0.00088 -0.00029 -0.00109 2.22469

A32 2.18770 -0.00069 -0.00211 -0.00697 -0.01161 2.17609

A33 2.03482 0.00016 0.00073 0.00239 0.00438 2.03920

A34 2.06066 0.00053 0.00138 0.00459 0.00723 2.06789

A35 2.16447 -0.00068 0.00322 0.00094 0.00605 2.17051

A36 2.18448 0.00049 -0.00172 -0.00254 -0.00603 2.17844

A37 1.93423 0.00019 -0.00150 0.00155 -0.00019 1.93405

A38 1.85680 -0.00004 0.00072 -0.00073 -0.00019 1.85661

A39 2.20014 0.00009 0.00006 0.00105 0.00119 2.20133

A40 2.22578 -0.00004 -0.00088 -0.00029 -0.00109 2.22469

A41 1.85680 -0.00004 0.00072 -0.00073 -0.00019 1.85661

A42 2.22578 -0.00004 -0.00088 -0.00029 -0.00109 2.22469

A43 2.20014 0.00009 0.00006 0.00105 0.00119 2.20133

A44 1.93423 0.00019 -0.00150 0.00155 -0.00019 1.93405

A45 2.16447 -0.00068 0.00322 0.00094 0.00605 2.17051

A46 2.18448 0.00049 -0.00172 -0.00254 -0.00603 2.17844

A47 1.84204 -0.00031 0.00133 -0.00225 -0.00044 1.84160

A48 2.18770 -0.00069 -0.00211 -0.00697 -0.01161 2.17609

A49 2.06066 0.00053 0.00138 0.00459 0.00723 2.06789

A50 2.03482 0.00016 0.00073 0.00239 0.00438 2.03920

A51 2.20671 0.00050 -0.00017 0.00363 0.00530 2.21201

A52 2.20740 -0.00011 -0.00007 -0.00351 -0.00539 2.20200

A53 1.86908 -0.00039 0.00024 -0.00011 -0.00001 1.86906

A54 1.88152 0.00043 -0.00080 0.00009 -0.00091 1.88061

A55 2.18493 -0.00021 0.00166 0.00069 0.00243 2.18737

A56 2.21635 -0.00021 -0.00097 -0.00077 -0.00166 2.21469

A57 1.88152 0.00043 -0.00080 0.00009 -0.00091 1.88061

A58 2.21635 -0.00021 -0.00097 -0.00077 -0.00166 2.21469

A59 2.18493 -0.00021 0.00166 0.00069 0.00243 2.18737

A60 1.86908 -0.00039 0.00024 -0.00011 -0.00001 1.86906

A61 2.20671 0.00050 -0.00017 0.00363 0.00530 2.21201

A62 2.20740 -0.00011 -0.00007 -0.00351 -0.00539 2.20200

A63 1.92294 -0.00008 0.00086 -0.00018 0.00111 1.92406

A64 2.18010 0.00004 -0.00036 0.00012 -0.00054 2.17956

A65 2.18010 0.00004 -0.00036 0.00012 -0.00054 2.17956

A66 2.18770 -0.00069 -0.00211 -0.00697 -0.01161 2.17609

A67 2.06066 0.00053 0.00138 0.00459 0.00723 2.06789

A68 2.03482 0.00016 0.00073 0.00239 0.00438 2.03920

A69 2.10367 0.00023 0.00081 0.00107 0.00187 2.10554

A70 2.09645 0.00048 0.00004 0.00194 0.00197 2.09842

A71 2.08306 -0.00071 -0.00084 -0.00301 -0.00384 2.07922

A72 2.09759 0.00046 0.00001 0.00183 0.00183 2.09942

A73 2.08776 -0.00019 -0.00044 -0.00083 -0.00129 2.08647

A74 2.09751 -0.00028 0.00034 -0.00101 -0.00068 2.09682

A75 2.09725 -0.00004 0.00021 -0.00017 0.00003 2.09728

A76 2.08879 0.00001 0.00051 0.00022 0.00073 2.08952

A77 2.09715 0.00002 -0.00072 -0.00004 -0.00076 2.09638

A78 2.09320 -0.00013 0.00035 -0.00017 0.00018 2.09338

A79 2.09504 0.00006 -0.00015 0.00008 -0.00008 2.09496

A80 2.09495 0.00007 -0.00020 0.00009 -0.00010 2.09484

A81 2.09729 -0.00004 0.00021 -0.00017 0.00004 2.09734

A82 2.09706 0.00002 -0.00074 -0.00007 -0.00081 2.09625

A83 2.08883 0.00001 0.00053 0.00024 0.00076 2.08959

A84 2.09765 0.00046 -0.00001 0.00180 0.00178 2.09943

A85 2.08717 -0.00020 -0.00043 -0.00091 -0.00135 2.08582

A86 2.09807 -0.00026 0.00035 -0.00091 -0.00058 2.09749

A87 2.09320 -0.00013 0.00035 -0.00017 0.00018 2.09338

A88 2.09504 0.00006 -0.00015 0.00008 -0.00008 2.09496

A89 2.09495 0.00007 -0.00020 0.00009 -0.00010 2.09484

A90 2.09725 -0.00004 0.00021 -0.00017 0.00003 2.09728

A91 2.09715 0.00002 -0.00072 -0.00004 -0.00076 2.09638

A92 2.08879 0.00001 0.00051 0.00022 0.00073 2.08952

A93 2.09759 0.00046 0.00001 0.00183 0.00183 2.09942

A94 2.09751 -0.00028 0.00034 -0.00101 -0.00068 2.09682

A95 2.08776 -0.00019 -0.00044 -0.00083 -0.00129 2.08647

A96 2.10367 0.00023 0.00081 0.00107 0.00187 2.10554

A97 2.09645 0.00048 0.00004 0.00194 0.00197 2.09842

A98 2.08306 -0.00071 -0.00084 -0.00301 -0.00384 2.07922

A99 2.09765 0.00046 -0.00001 0.00180 0.00178 2.09943

A100 2.08717 -0.00020 -0.00043 -0.00091 -0.00135 2.08582

A101 2.09807 -0.00026 0.00035 -0.00091 -0.00058 2.09749

A102 2.09729 -0.00004 0.00021 -0.00017 0.00004 2.09734

A103 2.09706 0.00002 -0.00074 -0.00007 -0.00081 2.09625

A104 2.08883 0.00001 0.00053 0.00024 0.00076 2.08959

A105 2.09645 0.00048 0.00004 0.00194 0.00197 2.09842

A106 2.10367 0.00023 0.00081 0.00107 0.00187 2.10554

A107 2.08306 -0.00071 -0.00084 -0.00301 -0.00384 2.07922

A108 2.09765 0.00046 -0.00001 0.00180 0.00178 2.09943

A109 2.08717 -0.00020 -0.00043 -0.00091 -0.00135 2.08582

A110 2.09807 -0.00026 0.00035 -0.00091 -0.00058 2.09749

A111 2.09729 -0.00004 0.00021 -0.00017 0.00004 2.09734

A112 2.08883 0.00001 0.00053 0.00024 0.00076 2.08959

A113 2.09706 0.00002 -0.00074 -0.00007 -0.00081 2.09625

A114 2.09320 -0.00013 0.00035 -0.00017 0.00018 2.09338

A115 2.09495 0.00007 -0.00020 0.00009 -0.00010 2.09484

A116 2.09504 0.00006 -0.00015 0.00008 -0.00008 2.09496

A117 2.09725 -0.00004 0.00021 -0.00017 0.00003 2.09728

A118 2.09715 0.00002 -0.00072 -0.00004 -0.00076 2.09638

A119 2.08879 0.00001 0.00051 0.00022 0.00073 2.08952

A120 2.09759 0.00046 0.00001 0.00183 0.00183 2.09942

A121 2.08776 -0.00019 -0.00044 -0.00083 -0.00129 2.08647

A122 2.09751 -0.00028 0.00034 -0.00101 -0.00068 2.09682

A123 2.09645 0.00048 0.00004 0.00194 0.00197 2.09842

A124 2.10367 0.00023 0.00081 0.00107 0.00187 2.10554

A125 2.08306 -0.00071 -0.00084 -0.00301 -0.00384 2.07922

A126 2.09765 0.00046 -0.00001 0.00180 0.00178 2.09943

A127 2.08717 -0.00020 -0.00043 -0.00091 -0.00135 2.08582

A128 2.09807 -0.00026 0.00035 -0.00091 -0.00058 2.09749

A129 2.09729 -0.00004 0.00021 -0.00017 0.00004 2.09734

A130 2.08883 0.00001 0.00053 0.00024 0.00076 2.08959

A131 2.09706 0.00002 -0.00074 -0.00007 -0.00081 2.09625

A132 2.09320 -0.00013 0.00035 -0.00017 0.00018 2.09338

A133 2.09495 0.00007 -0.00020 0.00009 -0.00010 2.09484

A134 2.09504 0.00006 -0.00015 0.00008 -0.00008 2.09496

A135 2.09725 -0.00004 0.00021 -0.00017 0.00003 2.09728

A136 2.09715 0.00002 -0.00072 -0.00004 -0.00076 2.09638

A137 2.08879 0.00001 0.00051 0.00022 0.00073 2.08952

A138 2.09759 0.00046 0.00001 0.00183 0.00183 2.09942

A139 2.08776 -0.00019 -0.00044 -0.00083 -0.00129 2.08647

A140 2.09751 -0.00028 0.00034 -0.00101 -0.00068 2.09682

D1 0.02008 0.00005 0.00605 0.00338 0.00933 0.02942

D2 -3.12234 0.00027 0.00565 0.01983 0.02531 -3.09703

D3 -3.09359 -0.00003 0.01120 0.00280 0.01400 -3.07958

D4 0.04717 0.00018 0.01080 0.01925 0.02998 0.07715

D5 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D6 -3.11302 -0.00009 0.00523 -0.00062 0.00468 -3.10835

D7 3.11302 0.00009 -0.00523 0.00062 -0.00468 3.10835

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 -0.03342 -0.00008 -0.01008 -0.00562 -0.01559 -0.04901

D10 3.09893 0.00001 -0.00239 0.00146 -0.00103 3.09790

D11 3.10901 -0.00030 -0.00968 -0.02209 -0.03146 3.07755

D12 -0.04183 -0.00021 -0.00199 -0.01500 -0.01690 -0.05873

D13 -2.99793 0.00013 0.02999 0.02294 0.05289 -2.94504

D14 0.14088 0.00016 0.03039 0.02513 0.05547 0.19635

D15 0.14268 0.00039 0.02951 0.04250 0.07181 0.21448

D16 -3.00170 0.00041 0.02991 0.04469 0.07439 -2.92731

D17 0.03342 0.00008 0.01008 0.00562 0.01559 0.04901

D18 -3.10901 0.00030 0.00968 0.02209 0.03146 -3.07755

D19 -3.09893 -0.00001 0.00239 -0.00146 0.00103 -3.09790

D20 0.04183 0.00021 0.00199 0.01500 0.01690 0.05873

D21 -0.02008 -0.00005 -0.00605 -0.00338 -0.00933 -0.02942

D22 3.09359 0.00003 -0.01120 -0.00280 -0.01400 3.07958

D23 3.12234 -0.00027 -0.00565 -0.01983 -0.02531 3.09703

D24 -0.04717 -0.00018 -0.01080 -0.01925 -0.02998 -0.07715

D25 -0.14268 -0.00039 -0.02951 -0.04250 -0.07181 -0.21448

D26 3.00170 -0.00041 -0.02991 -0.04469 -0.07439 2.92731

D27 2.99793 -0.00013 -0.02999 -0.02294 -0.05289 2.94504

D28 -0.14088 -0.00016 -0.03039 -0.02513 -0.05547 -0.19635

D29 -0.14383 -0.00031 -0.02437 -0.03634 -0.06048 -0.20431

D30 3.00187 -0.00019 -0.02163 -0.02056 -0.04216 2.95971

D31 2.99493 -0.00028 -0.02396 -0.03412 -0.05786 2.93707

D32 -0.14255 -0.00017 -0.02123 -0.01834 -0.03954 -0.18209

D33 -0.99132 -0.00002 0.03590 0.03795 0.07386 -0.91746

D34 2.15203 -0.00005 0.03698 0.03642 0.07342 2.22545

D35 2.15285 -0.00004 0.03553 0.03595 0.07147 2.22432

D36 -0.98698 -0.00007 0.03662 0.03442 0.07103 -0.91595

D37 -3.10429 0.00040 0.00967 0.02955 0.03887 -3.06542

D38 0.03366 0.00029 0.00724 0.01556 0.02271 0.05637

D39 3.11677 -0.00029 -0.00695 -0.02364 -0.03042 3.08635

D40 -0.05571 -0.00019 -0.01075 -0.02273 -0.03340 -0.08911

D41 -0.02123 -0.00019 -0.00455 -0.00983 -0.01432 -0.03555

D42 3.08947 -0.00009 -0.00836 -0.00892 -0.01730 3.07218

D43 -0.03366 -0.00029 -0.00724 -0.01556 -0.02271 -0.05637

D44 3.10429 -0.00040 -0.00967 -0.02955 -0.03887 3.06542

D45 0.02123 0.00019 0.00455 0.00983 0.01432 0.03555

D46 -3.08947 0.00009 0.00836 0.00892 0.01730 -3.07218

D47 -3.11677 0.00029 0.00695 0.02364 0.03042 -3.08635

D48 0.05571 0.00019 0.01075 0.02273 0.03340 0.08911

D49 0.14383 0.00031 0.02437 0.03634 0.06048 0.20431

D50 -2.99493 0.00028 0.02396 0.03412 0.05786 -2.93707

D51 -3.00187 0.00019 0.02163 0.02056 0.04216 -2.95971

D52 0.14255 0.00017 0.02123 0.01834 0.03954 0.18209

D53 0.00000 0.00000 -0.00000 -0.00000 0.00000 0.00000

D54 -3.11010 -0.00011 0.00386 -0.00096 0.00298 -3.10712

D55 3.11010 0.00011 -0.00386 0.00096 -0.00298 3.10712

D56 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D57 -3.00187 0.00019 0.02163 0.02056 0.04216 -2.95971

D58 0.14383 0.00031 0.02437 0.03634 0.06048 0.20431

D59 0.14255 0.00017 0.02123 0.01834 0.03954 0.18209

D60 -2.99493 0.00028 0.02396 0.03412 0.05786 -2.93707

D61 0.99132 0.00002 -0.03590 -0.03795 -0.07386 0.91746

D62 -2.15203 0.00005 -0.03698 -0.03642 -0.07342 -2.22545

D63 -2.15285 0.00004 -0.03553 -0.03595 -0.07147 -2.22432

D64 0.98698 0.00007 -0.03662 -0.03442 -0.07103 0.91595

D65 -3.11677 0.00029 0.00695 0.02364 0.03042 -3.08635

D66 0.05571 0.00019 0.01075 0.02273 0.03340 0.08911

D67 0.02123 0.00019 0.00455 0.00983 0.01432 0.03555

D68 -3.08947 0.00009 0.00836 0.00892 0.01730 -3.07218

D69 3.10429 -0.00040 -0.00967 -0.02955 -0.03887 3.06542

D70 -0.03366 -0.00029 -0.00724 -0.01556 -0.02271 -0.05637

D71 0.00000 0.00000 -0.00000 -0.00000 0.00000 0.00000

D72 -3.11010 -0.00011 0.00386 -0.00096 0.00298 -3.10712

D73 3.11010 0.00011 -0.00386 0.00096 -0.00298 3.10712

D74 0.00000 -0.00000 0.00000 0.00000 -0.00000 0.00000

D75 -0.02123 -0.00019 -0.00455 -0.00983 -0.01432 -0.03555

D76 3.11677 -0.00029 -0.00695 -0.02364 -0.03042 3.08635

D77 3.08947 -0.00009 -0.00836 -0.00892 -0.01730 3.07218

D78 -0.05571 -0.00019 -0.01075 -0.02273 -0.03340 -0.08911

D79 0.03366 0.00029 0.00724 0.01556 0.02271 0.05637

D80 -3.10429 0.00040 0.00967 0.02955 0.03887 -3.06542

D81 3.00187 -0.00019 -0.02163 -0.02056 -0.04216 2.95971

D82 -0.14255 -0.00017 -0.02123 -0.01834 -0.03954 -0.18209

D83 -0.14383 -0.00031 -0.02437 -0.03634 -0.06048 -0.20431

D84 2.99493 -0.00028 -0.02396 -0.03412 -0.05786 2.93707

D85 2.99793 -0.00013 -0.02999 -0.02294 -0.05289 2.94504

D86 -0.14268 -0.00039 -0.02951 -0.04250 -0.07181 -0.21448

D87 -0.14088 -0.00016 -0.03039 -0.02513 -0.05547 -0.19635

D88 3.00170 -0.00041 -0.02991 -0.04469 -0.07439 2.92731

D89 -0.98698 -0.00007 0.03662 0.03442 0.07103 -0.91595

D90 2.15285 -0.00004 0.03553 0.03595 0.07147 2.22432

D91 2.15203 -0.00005 0.03698 0.03642 0.07342 2.22545

D92 -0.99132 -0.00002 0.03590 0.03795 0.07386 -0.91746

D93 3.12234 -0.00027 -0.00565 -0.01983 -0.02531 3.09703

D94 -0.04717 -0.00018 -0.01080 -0.01925 -0.02998 -0.07715

D95 -0.02008 -0.00005 -0.00605 -0.00338 -0.00933 -0.02942

D96 3.09359 0.00003 -0.01120 -0.00280 -0.01400 3.07958

D97 -3.10901 0.00030 0.00968 0.02209 0.03146 -3.07755

D98 0.04183 0.00021 0.00199 0.01500 0.01690 0.05873

D99 0.03342 0.00008 0.01008 0.00562 0.01559 0.04901

D100 -3.09893 -0.00001 0.00239 -0.00146 0.00103 -3.09790

D101 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D102 3.11302 0.00009 -0.00523 0.00062 -0.00468 3.10835

D103 -3.11302 -0.00009 0.00523 -0.00062 0.00468 -3.10835

D104 0.00000 0.00000 0.00000 0.00000 -0.00000 0.00000

D105 0.02008 0.00005 0.00605 0.00338 0.00933 0.02942

D106 -3.12234 0.00027 0.00565 0.01983 0.02531 -3.09703

D107 -3.09359 -0.00003 0.01120 0.00280 0.01400 -3.07958

D108 0.04717 0.00018 0.01080 0.01925 0.02998 0.07715

D109 -0.03342 -0.00008 -0.01008 -0.00562 -0.01559 -0.04901

D110 3.09893 0.00001 -0.00239 0.00146 -0.00103 3.09790

D111 3.10901 -0.00030 -0.00968 -0.02209 -0.03146 3.07755

D112 -0.04183 -0.00021 -0.00199 -0.01500 -0.01690 -0.05873

D113 -2.99793 0.00013 0.02999 0.02294 0.05289 -2.94504

D114 0.14088 0.00016 0.03039 0.02513 0.05547 0.19635

D115 0.14268 0.00039 0.02951 0.04250 0.07181 0.21448

D116 -3.00170 0.00041 0.02991 0.04469 0.07439 -2.92731

D117 0.98698 0.00007 -0.03662 -0.03442 -0.07103 0.91595

D118 -2.15285 0.00004 -0.03553 -0.03595 -0.07147 -2.22432

D119 -2.15203 0.00005 -0.03698 -0.03642 -0.07342 -2.22545

D120 0.99132 0.00002 -0.03590 -0.03795 -0.07386 0.91746

D121 -3.12873 -0.00007 0.00232 -0.00249 -0.00017 -3.12891

D122 -0.01472 -0.00004 -0.00262 -0.00317 -0.00578 -0.02051

D123 0.01111 -0.00004 0.00124 -0.00097 0.00027 0.01138

D124 3.12512 -0.00001 -0.00370 -0.00165 -0.00534 3.11978

D125 -3.13205 -0.00004 0.00090 -0.00146 -0.00055 -3.13260

D126 -0.01641 -0.00001 -0.00446 -0.00213 -0.00659 -0.02300

D127 0.01128 -0.00007 0.00198 -0.00297 -0.00100 0.01029

D128 3.12693 -0.00004 -0.00339 -0.00365 -0.00703 3.11989

D129 -0.02241 0.00011 -0.00306 0.00362 0.00056 -0.02185

D130 3.11956 0.00007 -0.00409 0.00193 -0.00216 3.11740

D131 -3.13627 0.00008 0.00191 0.00430 0.00622 -3.13005

D132 0.00571 0.00004 0.00088 0.00261 0.00350 0.00920

D133 0.01129 -0.00007 0.00166 -0.00234 -0.00068 0.01061

D134 -3.13032 -0.00006 0.00171 -0.00202 -0.00031 -3.13063

D135 -3.13069 -0.00003 0.00270 -0.00064 0.00205 -3.12863

D136 0.01089 -0.00003 0.00274 -0.00032 0.00242 0.01331

D137 0.01117 -0.00006 0.00157 -0.00164 -0.00007 0.01110

D138 -3.13093 -0.00002 0.00275 0.00015 0.00289 -3.12804

D139 -3.13041 -0.00006 0.00152 -0.00196 -0.00044 -3.13085

D140 0.01067 -0.00003 0.00270 -0.00017 0.00253 0.01320

D141 -0.02244 0.00012 -0.00339 0.00428 0.00090 -0.02154

D142 -3.13792 0.00008 0.00202 0.00496 0.00699 -3.13093

D143 3.11966 0.00009 -0.00456 0.00251 -0.00205 3.11760

D144 0.00418 0.00005 0.00085 0.00319 0.00404 0.00821

D145 -0.01129 0.00007 -0.00166 0.00234 0.00068 -0.01061

D146 3.13069 0.00003 -0.00270 0.00064 -0.00205 3.12863

D147 3.13032 0.00006 -0.00171 0.00202 0.00031 3.13063

D148 -0.01089 0.00003 -0.00274 0.00032 -0.00242 -0.01331

D149 -0.01117 0.00006 -0.00157 0.00164 0.00007 -0.01110

D150 3.13093 0.00002 -0.00275 -0.00015 -0.00289 3.12804

D151 3.13041 0.00006 -0.00152 0.00196 0.00044 3.13085

D152 -0.01067 0.00003 -0.00270 0.00017 -0.00253 -0.01320

D153 0.02241 -0.00011 0.00306 -0.00362 -0.00056 0.02185

D154 3.13627 -0.00008 -0.00191 -0.00430 -0.00622 3.13005

D155 -3.11956 -0.00007 0.00409 -0.00193 0.00216 -3.11740

D156 -0.00571 -0.00004 -0.00088 -0.00261 -0.00350 -0.00920

D157 3.12873 0.00007 -0.00232 0.00249 0.00017 3.12891

D158 -0.01111 0.00004 -0.00124 0.00097 -0.00027 -0.01138

D159 0.01472 0.00004 0.00262 0.00317 0.00578 0.02051

D160 -3.12512 0.00001 0.00370 0.00165 0.00534 -3.11978

D161 3.13205 0.00004 -0.00090 0.00146 0.00055 3.13260

D162 0.01641 0.00001 0.00446 0.00213 0.00659 0.02300

D163 -0.01128 0.00007 -0.00198 0.00297 0.00100 -0.01029

D164 -3.12693 0.00004 0.00339 0.00365 0.00703 -3.11989

D165 0.02244 -0.00012 0.00339 -0.00428 -0.00090 0.02154

D166 -3.11966 -0.00009 0.00456 -0.00251 0.00205 -3.11760

D167 3.13792 -0.00008 -0.00202 -0.00496 -0.00699 3.13093

D168 -0.00418 -0.00005 -0.00085 -0.00319 -0.00404 -0.00821

D169 3.13205 0.00004 -0.00090 0.00146 0.00055 3.13260

D170 0.01641 0.00001 0.00446 0.00213 0.00659 0.02300

D171 -0.01128 0.00007 -0.00198 0.00297 0.00100 -0.01029

D172 -3.12693 0.00004 0.00339 0.00365 0.00703 -3.11989

D173 3.12873 0.00007 -0.00232 0.00249 0.00017 3.12891

D174 0.01472 0.00004 0.00262 0.00317 0.00578 0.02051

D175 -0.01111 0.00004 -0.00124 0.00097 -0.00027 -0.01138

D176 -3.12512 0.00001 0.00370 0.00165 0.00534 -3.11978

D177 0.02244 -0.00012 0.00339 -0.00428 -0.00090 0.02154

D178 -3.11966 -0.00009 0.00456 -0.00251 0.00205 -3.11760

D179 3.13792 -0.00008 -0.00202 -0.00496 -0.00699 3.13093

D180 -0.00418 -0.00005 -0.00085 -0.00319 -0.00404 -0.00821

D181 -0.01117 0.00006 -0.00157 0.00164 0.00007 -0.01110

D182 3.13041 0.00006 -0.00152 0.00196 0.00044 3.13085

D183 3.13093 0.00002 -0.00275 -0.00015 -0.00289 3.12804

D184 -0.01067 0.00003 -0.00270 0.00017 -0.00253 -0.01320

D185 -0.01129 0.00007 -0.00166 0.00234 0.00068 -0.01061

D186 3.13069 0.00003 -0.00270 0.00064 -0.00205 3.12863

D187 3.13032 0.00006 -0.00171 0.00202 0.00031 3.13063

D188 -0.01089 0.00003 -0.00274 0.00032 -0.00242 -0.01331

D189 0.02241 -0.00011 0.00306 -0.00362 -0.00056 0.02185

D190 3.13627 -0.00008 -0.00191 -0.00430 -0.00622 3.13005

D191 -3.11956 -0.00007 0.00409 -0.00193 0.00216 -3.11740

D192 -0.00571 -0.00004 -0.00088 -0.00261 -0.00350 -0.00920

D193 -3.13205 -0.00004 0.00090 -0.00146 -0.00055 -3.13260

D194 -0.01641 -0.00001 -0.00446 -0.00213 -0.00659 -0.02300

D195 0.01128 -0.00007 0.00198 -0.00297 -0.00100 0.01029

D196 3.12693 -0.00004 -0.00339 -0.00365 -0.00703 3.11989

D197 -3.12873 -0.00007 0.00232 -0.00249 -0.00017 -3.12891

D198 -0.01472 -0.00004 -0.00262 -0.00317 -0.00578 -0.02051

D199 0.01111 -0.00004 0.00124 -0.00097 0.00027 0.01138

D200 3.12512 -0.00001 -0.00370 -0.00165 -0.00534 3.11978

D201 -0.02244 0.00012 -0.00339 0.00428 0.00090 -0.02154

D202 3.11966 0.00009 -0.00456 0.00251 -0.00205 3.11760

D203 -3.13792 0.00008 0.00202 0.00496 0.00699 -3.13093

D204 0.00418 0.00005 0.00085 0.00319 0.00404 0.00821

D205 0.01117 -0.00006 0.00157 -0.00164 -0.00007 0.01110

D206 -3.13041 -0.00006 0.00152 -0.00196 -0.00044 -3.13085

D207 -3.13093 -0.00002 0.00275 0.00015 0.00289 -3.12804

D208 0.01067 -0.00003 0.00270 -0.00017 0.00253 0.01320

D209 0.01129 -0.00007 0.00166 -0.00234 -0.00068 0.01061

D210 -3.13069 -0.00003 0.00270 -0.00064 0.00205 -3.12863

D211 -3.13032 -0.00006 0.00171 -0.00202 -0.00031 -3.13063

D212 0.01089 -0.00003 0.00274 -0.00032 0.00242 0.01331

D213 -0.02241 0.00011 -0.00306 0.00362 0.00056 -0.02185

D214 -3.13627 0.00008 0.00191 0.00430 0.00622 -3.13005

D215 3.11956 0.00007 -0.00409 0.00193 -0.00216 3.11740

D216 0.00571 0.00004 0.00088 0.00261 0.00350 0.00920

Item Value Threshold Converged?

Maximum Force 0.002596 0.000450 NO

RMS Force 0.000387 0.000300 NO

Maximum Displacement 0.559922 0.001800 NO

RMS Displacement 0.148957 0.001200 NO

Predicted change in Energy=-3.923321D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Aug 18 14:07:14 2019, MaxMem= 2013265920 cpu: 1.4

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

Stoichiometry C44H30N4(1+,2)

Framework group C2V[SGV(H2N2),SGV'(N2),X(C44H28)]

Deg. of freedom 59

Full point group C2V NOp 4

RotChk: IX=0 Diff= 1.55D-16

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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1 6 0 -0.689447 4.143826 0.596441

2 6 0 -1.123092 2.853360 0.184486

3 7 0 0.000000 2.096743 -0.016645

4 6 0 1.123092 2.853360 0.184486

5 6 0 0.689447 4.143826 0.596441

6 6 0 2.464186 2.428485 -0.004337

7 6 0 2.862750 1.088157 -0.192843

8 7 0 2.059337 -0.000000 0.004173

9 6 0 2.862750 -1.088157 -0.192843

10 6 0 4.197061 -0.678308 -0.598872

11 6 0 4.197061 0.678308 -0.598872

12 6 0 -2.464186 2.428485 -0.004337

13 6 0 -2.862750 1.088157 -0.192843

14 6 0 -4.197061 0.678308 -0.598872

15 6 0 -4.197061 -0.678308 -0.598872

16 6 0 -2.862750 -1.088157 -0.192843

17 7 0 -2.059337 0.000000 0.004173

18 6 0 -2.464186 -2.428485 -0.004337

19 6 0 -1.123092 -2.853360 0.184486

20 6 0 -0.689447 -4.143826 0.596441

21 6 0 0.689447 -4.143826 0.596441

22 6 0 1.123092 -2.853360 0.184486

23 7 0 -0.000000 -2.096743 -0.016645

24 6 0 2.464186 -2.428485 -0.004337

25 6 0 3.504206 3.479363 0.000028

26 6 0 3.390629 4.602039 -0.835679

27 6 0 4.380636 5.578684 -0.836676

28 6 0 5.480677 5.462102 0.012073

29 6 0 5.595306 4.357194 0.855213

30 6 0 4.621893 3.364452 0.842337

31 6 0 -5.480677 5.462102 0.012073

32 6 0 -4.380636 5.578684 -0.836676

33 6 0 -3.390629 4.602039 -0.835679

34 6 0 -3.504206 3.479363 0.000028

35 6 0 -4.621893 3.364452 0.842337

36 6 0 -5.595306 4.357194 0.855213

37 6 0 3.504206 -3.479363 0.000028

38 6 0 4.621893 -3.364452 0.842337

39 6 0 5.595306 -4.357194 0.855213

40 6 0 5.480677 -5.462102 0.012073

41 6 0 4.380636 -5.578684 -0.836676

42 6 0 3.390629 -4.602039 -0.835679

43 6 0 -3.504206 -3.479363 0.000028

44 6 0 -4.621893 -3.364452 0.842337

45 6 0 -5.595306 -4.357194 0.855213

46 6 0 -5.480677 -5.462102 0.012073

47 6 0 -4.380636 -5.578684 -0.836676

48 6 0 -3.390629 -4.602039 -0.835679

49 1 0 -1.335975 4.955202 0.885512

50 1 0 1.335975 4.955202 0.885512

51 1 0 5.006779 -1.334208 -0.876098

52 1 0 5.006779 1.334208 -0.876098

53 1 0 -5.006779 1.334208 -0.876098

54 1 0 -5.006779 -1.334208 -0.876098

55 1 0 -1.335975 -4.955202 0.885512

56 1 0 1.335975 -4.955202 0.885512

57 1 0 2.541522 4.687586 -1.502911

58 1 0 4.294711 6.430727 -1.502173

59 1 0 6.246499 6.230259 0.016848

60 1 0 6.443445 4.270051 1.525533

61 1 0 4.705684 2.511101 1.504192

62 1 0 -6.246499 6.230259 0.016848

63 1 0 -4.294711 6.430727 -1.502173

64 1 0 -2.541522 4.687586 -1.502911

65 1 0 -4.705684 2.511101 1.504192

66 1 0 -6.443445 4.270051 1.525533

67 1 0 4.705684 -2.511101 1.504192

68 1 0 6.443445 -4.270051 1.525533

69 1 0 6.246499 -6.230259 0.016848

70 1 0 4.294711 -6.430727 -1.502173

71 1 0 2.541522 -4.687586 -1.502911

72 1 0 -4.705684 -2.511101 1.504192

73 1 0 -6.443445 -4.270051 1.525533

74 1 0 -6.246499 -6.230259 0.016848

75 1 0 -4.294711 -6.430727 -1.502173

76 1 0 -2.541522 -4.687586 -1.502911

77 1 0 0.000000 1.121129 -0.280549

78 1 0 -0.000000 -1.121129 -0.280549

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

Rotational constants (GHZ): 0.0593526 0.0587341 0.0302892

Leave Link 202 at Sun Aug 18 14:07:14 2019, MaxMem= 2013265920 cpu: 0.0

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

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

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

There are 261 symmetry adapted cartesian basis functions of A1 symmetry.

There are 240 symmetry adapted cartesian basis functions of A2 symmetry.

There are 249 symmetry adapted cartesian basis functions of B1 symmetry.

There are 252 symmetry adapted cartesian basis functions of B2 symmetry.

There are 248 symmetry adapted basis functions of A1 symmetry.

There are 229 symmetry adapted basis functions of A2 symmetry.

There are 237 symmetry adapted basis functions of B1 symmetry.

There are 240 symmetry adapted basis functions of B2 symmetry.

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

161 alpha electrons 160 beta electrons

nuclear repulsion energy 5373.9633136736 Hartrees.

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

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

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

NAtoms= 78 NActive= 78 NUniq= 21 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=T Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2129225246 Hartrees.

Nuclear repulsion after empirical dispersion term = 5373.7503911490 Hartrees.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 78

GePol: Total number of spheres = 78

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

GePol: Number of points = 5722

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.28D-11

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 366

GePol: Fraction of low-weight points (<1% of avg) = 6.40%

GePol: Cavity surface area = 607.726 Ang\*\*2

GePol: Cavity volume = 626.946 Ang\*\*3

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

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PCM non-electrostatic energy = -0.0022658303 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5373.7481253186 Hartrees.

Leave Link 301 at Sun Aug 18 14:07:14 2019, MaxMem= 2013265920 cpu: 1.0

(Enter /home/kira/g09/l302.exe)

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

NBasis= 954 RedAO= T EigKep= 6.43D-05 NBF= 248 229 237 240

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 248 229 237 240

Precomputing XC quadrature grid using

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

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

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

Leave Link 302 at Sun Aug 18 14:07:15 2019, MaxMem= 2013265920 cpu: 9.5

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

DipDrv: MaxL=1.

Leave Link 303 at Sun Aug 18 14:07:15 2019, MaxMem= 2013265920 cpu: 1.3

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

Initial guess from the checkpoint file: "TPPcation.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-A1.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7878 S= 0.5187

Generating alternative initial guess.

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -1914.08927468079

Leave Link 401 at Sun Aug 18 14:07:21 2019, MaxMem= 2013265920 cpu: 44.4

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3049894 IEndB= 3049894 NGot= 2013265920 MDV= 2011237673

LenX= 2011237673 LenY= 2010232667

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

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

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

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

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

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 98223852.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.11D-15 for 5709.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.44D-15 for 4808 4707.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.88D-15 for 5709.

Iteration 1 A^-1\*A deviation from orthogonality is 1.62D-12 for 4011 4009.

E= -1914.03138328077

DIIS: error= 1.46D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.03138328077 IErMin= 1 ErrMin= 1.46D-02

ErrMax= 1.46D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.14D-01 BMatP= 3.14D-01

IDIUse=3 WtCom= 8.54D-01 WtEn= 1.46D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Recover alternate guess density for next cycle.

RMSDP=1.08D-03 MaxDP=5.20D-02 OVMax= 0.00D+00

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.07D-03 CP: 9.92D-01

E= -1913.31363159443 Delta-E= 0.717751686341 Rises=F Damp=F

Switch densities from cycles 1 and 2 for lowest energy.

DIIS: error= 4.52D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 1 EnMin= -1914.03138328077 IErMin= 1 ErrMin= 1.46D-02

ErrMax= 4.52D-02 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.79D+00 BMatP= 3.14D-01

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

Coeff-Com: 0.925D+00 0.753D-01

Coeff: 0.925D+00 0.753D-01

Gap= 0.498 Goal= None Shift= 0.000

Gap= 0.513 Goal= None Shift= 0.000

RMSDP=5.35D-03 MaxDP=3.32D-01 DE= 7.18D-01 OVMax= 6.62D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.80D-04 CP: 9.96D-01 9.71D-02

E= -1914.19332906722 Delta-E= -0.879697472791 Rises=F Damp=F

DIIS: error= 2.79D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.19332906722 IErMin= 3 ErrMin= 2.79D-03

ErrMax= 2.79D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.32D-02 BMatP= 3.14D-01

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

Coeff-Com: -0.441D-01 0.615D-01 0.983D+00

Coeff: -0.441D-01 0.615D-01 0.983D+00

Gap= 0.094 Goal= None Shift= 0.000

Gap= 0.057 Goal= None Shift= 0.000

RMSDP=1.17D-04 MaxDP=4.25D-03 DE=-8.80D-01 OVMax= 2.49D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 9.13D-05 CP: 9.95D-01 1.65D-01 9.92D-01

E= -1914.19913030591 Delta-E= -0.005801238693 Rises=F Damp=F

DIIS: error= 1.25D-03 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.19913030591 IErMin= 4 ErrMin= 1.25D-03

ErrMax= 1.25D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 6.39D-03 BMatP= 2.32D-02

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

Coeff-Com: -0.317D-01 0.182D-01 0.451D+00 0.562D+00

Coeff: -0.317D-01 0.182D-01 0.451D+00 0.562D+00

Gap= 0.094 Goal= None Shift= 0.000

Gap= 0.057 Goal= None Shift= 0.000

RMSDP=5.31D-05 MaxDP=2.77D-03 DE=-5.80D-03 OVMax= 1.67D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.38D-05 CP: 9.95D-01 1.56D-01 1.02D+00 5.88D-01

E= -1914.20057902090 Delta-E= -0.001448714988 Rises=F Damp=F

DIIS: error= 4.41D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.20057902090 IErMin= 5 ErrMin= 4.41D-04

ErrMax= 4.41D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 8.74D-04 BMatP= 6.39D-03

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

Coeff-Com: -0.113D-01 0.247D-02 0.127D+00 0.312D+00 0.569D+00

Coeff: -0.113D-01 0.247D-02 0.127D+00 0.312D+00 0.569D+00

Gap= 0.093 Goal= None Shift= 0.000

Gap= 0.058 Goal= None Shift= 0.000

RMSDP=1.90D-05 MaxDP=9.73D-04 DE=-1.45D-03 OVMax= 5.03D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.32D-05 CP: 9.95D-01 1.57D-01 1.03D+00 6.60D-01 6.59D-01

E= -1914.20078999061 Delta-E= -0.000210969710 Rises=F Damp=F

DIIS: error= 1.94D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.20078999061 IErMin= 6 ErrMin= 1.94D-04

ErrMax= 1.94D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 9.35D-05 BMatP= 8.74D-04

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

Coeff-Com: -0.335D-02-0.345D-03 0.268D-01 0.117D+00 0.315D+00 0.545D+00

Coeff: -0.335D-02-0.345D-03 0.268D-01 0.117D+00 0.315D+00 0.545D+00

Gap= 0.093 Goal= None Shift= 0.000

Gap= 0.058 Goal= None Shift= 0.000

RMSDP=7.28D-06 MaxDP=4.97D-04 DE=-2.11D-04 OVMax= 2.37D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 4.39D-06 CP: 9.95D-01 1.56D-01 1.03D+00 6.79D-01 6.97D-01

CP: 6.02D-01

E= -1914.20081149593 Delta-E= -0.000021505316 Rises=F Damp=F

DIIS: error= 6.53D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.20081149593 IErMin= 7 ErrMin= 6.53D-05

ErrMax= 6.53D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.17D-05 BMatP= 9.35D-05

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

Coeff-Com: -0.321D-03-0.462D-03-0.328D-02 0.183D-01 0.904D-01 0.297D+00

Coeff-Com: 0.598D+00

Coeff: -0.321D-03-0.462D-03-0.328D-02 0.183D-01 0.904D-01 0.297D+00

Coeff: 0.598D+00

Gap= 0.093 Goal= None Shift= 0.000

Gap= 0.058 Goal= None Shift= 0.000

RMSDP=2.71D-06 MaxDP=2.09D-04 DE=-2.15D-05 OVMax= 8.73D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.62D-06 CP: 9.95D-01 1.56D-01 1.03D+00 6.80D-01 7.11D-01

CP: 7.14D-01 6.77D-01

E= -1914.20081443096 Delta-E= -0.000002935035 Rises=F Damp=F

DIIS: error= 3.29D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.20081443096 IErMin= 8 ErrMin= 3.29D-05

ErrMax= 3.29D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.31D-06 BMatP= 1.17D-05

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

Coeff-Com: 0.215D-03-0.229D-03-0.548D-02-0.389D-02 0.148D-01 0.110D+00

Coeff-Com: 0.356D+00 0.529D+00

Coeff: 0.215D-03-0.229D-03-0.548D-02-0.389D-02 0.148D-01 0.110D+00

Coeff: 0.356D+00 0.529D+00

Gap= 0.093 Goal= None Shift= 0.000

Gap= 0.058 Goal= None Shift= 0.000

RMSDP=1.01D-06 MaxDP=6.60D-05 DE=-2.94D-06 OVMax= 3.47D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 7.77D-07 CP: 9.95D-01 1.56D-01 1.03D+00 6.80D-01 7.17D-01

CP: 7.07D-01 7.66D-01 7.52D-01

E= -1914.20081514044 Delta-E= -0.000000709482 Rises=F Damp=F

DIIS: error= 1.49D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.20081514044 IErMin= 9 ErrMin= 1.49D-05

ErrMax= 1.49D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.61D-07 BMatP= 2.31D-06

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

Coeff-Com: 0.160D-03 0.302D-04-0.139D-02-0.585D-02-0.157D-01-0.271D-01

Coeff-Com: -0.177D-02 0.201D+00 0.851D+00

Coeff: 0.160D-03 0.302D-04-0.139D-02-0.585D-02-0.157D-01-0.271D-01

Coeff: -0.177D-02 0.201D+00 0.851D+00

Gap= 0.093 Goal= None Shift= 0.000

Gap= 0.058 Goal= None Shift= 0.000

RMSDP=5.57D-07 MaxDP=3.10D-05 DE=-7.09D-07 OVMax= 1.77D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 3.01D-07 CP: 9.95D-01 1.56D-01 1.03D+00 6.81D-01 7.18D-01

CP: 7.21D-01 7.98D-01 9.73D-01 1.22D+00

E= -1914.20081536780 Delta-E= -0.000000227351 Rises=F Damp=F

DIIS: error= 1.02D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.20081536780 IErMin=10 ErrMin= 1.02D-05

ErrMax= 1.02D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 6.92D-08 BMatP= 2.61D-07

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

Coeff-Com: -0.240D-05 0.601D-04 0.103D-02-0.764D-03-0.848D-02-0.351D-01

Coeff-Com: -0.917D-01-0.738D-01 0.238D+00 0.971D+00

Coeff: -0.240D-05 0.601D-04 0.103D-02-0.764D-03-0.848D-02-0.351D-01

Coeff: -0.917D-01-0.738D-01 0.238D+00 0.971D+00

Gap= 0.093 Goal= None Shift= 0.000

Gap= 0.058 Goal= None Shift= 0.000

RMSDP=4.01D-07 MaxDP=2.52D-05 DE=-2.27D-07 OVMax= 1.36D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.86D-07 CP: 9.95D-01 1.56D-01 1.03D+00 6.81D-01 7.19D-01

CP: 7.24D-01 8.25D-01 1.10D+00 1.53D+00 1.35D+00

E= -1914.20081545601 Delta-E= -0.000000088217 Rises=F Damp=F

DIIS: error= 7.29D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.20081545601 IErMin=11 ErrMin= 7.29D-06

ErrMax= 7.29D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.71D-08 BMatP= 6.92D-08

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

Coeff-Com: -0.635D-04 0.234D-04 0.121D-02 0.182D-02 0.104D-02-0.109D-01

Coeff-Com: -0.584D-01-0.126D+00-0.198D+00 0.619D+00 0.770D+00

Coeff: -0.635D-04 0.234D-04 0.121D-02 0.182D-02 0.104D-02-0.109D-01

Coeff: -0.584D-01-0.126D+00-0.198D+00 0.619D+00 0.770D+00

Gap= 0.093 Goal= None Shift= 0.000

Gap= 0.058 Goal= None Shift= 0.000

RMSDP=2.61D-07 MaxDP=1.28D-05 DE=-8.82D-08 OVMax= 9.07D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 9.54D-08 CP: 9.95D-01 1.56D-01 1.03D+00 6.81D-01 7.19D-01

CP: 7.27D-01 8.36D-01 1.17D+00 1.73D+00 1.77D+00

CP: 1.08D+00

E= -1914.20081548668 Delta-E= -0.000000030671 Rises=F Damp=F

DIIS: error= 1.94D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.20081548668 IErMin=12 ErrMin= 1.94D-06

ErrMax= 1.94D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.15D-09 BMatP= 3.71D-08

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

Coeff-Com: -0.179D-04-0.427D-05 0.215D-03 0.655D-03 0.159D-02 0.168D-02

Coeff-Com: -0.608D-02-0.261D-01-0.914D-01 0.553D-01 0.232D+00 0.833D+00

Coeff: -0.179D-04-0.427D-05 0.215D-03 0.655D-03 0.159D-02 0.168D-02

Coeff: -0.608D-02-0.261D-01-0.914D-01 0.553D-01 0.232D+00 0.833D+00

Gap= 0.093 Goal= None Shift= 0.000

Gap= 0.058 Goal= None Shift= 0.000

RMSDP=7.43D-08 MaxDP=3.12D-06 DE=-3.07D-08 OVMax= 2.43D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 4.36D-08 CP: 9.95D-01 1.56D-01 1.03D+00 6.81D-01 7.19D-01

CP: 7.28D-01 8.38D-01 1.18D+00 1.77D+00 1.88D+00

CP: 1.25D+00 1.14D+00

E= -1914.20081548974 Delta-E= -0.000000003060 Rises=F Damp=F

DIIS: error= 9.55D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1914.20081548974 IErMin=13 ErrMin= 9.55D-07

ErrMax= 9.55D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.38D-09 BMatP= 3.15D-09

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

Coeff-Com: 0.708D-05-0.744D-05-0.210D-03-0.146D-03 0.536D-03 0.371D-02

Coeff-Com: 0.121D-01 0.214D-01 0.619D-02-0.138D+00-0.878D-01 0.435D+00

Coeff-Com: 0.748D+00

Coeff: 0.708D-05-0.744D-05-0.210D-03-0.146D-03 0.536D-03 0.371D-02

Coeff: 0.121D-01 0.214D-01 0.619D-02-0.138D+00-0.878D-01 0.435D+00

Coeff: 0.748D+00

Gap= 0.093 Goal= None Shift= 0.000

Gap= 0.058 Goal= None Shift= 0.000

RMSDP=4.15D-08 MaxDP=1.76D-06 DE=-3.06D-09 OVMax= 1.36D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 2.14D-08 CP: 9.95D-01 1.56D-01 1.03D+00 6.81D-01 7.19D-01

CP: 7.28D-01 8.38D-01 1.19D+00 1.78D+00 1.92D+00

CP: 1.33D+00 1.41D+00 1.19D+00

E= -1914.20081549086 Delta-E= -0.000000001115 Rises=F Damp=F

DIIS: error= 6.50D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1914.20081549086 IErMin=14 ErrMin= 6.50D-07

ErrMax= 6.50D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.82D-10 BMatP= 1.38D-09

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

Coeff-Com: 0.849D-05-0.170D-06-0.149D-03-0.276D-03-0.416D-03 0.711D-03

Coeff-Com: 0.661D-02 0.170D-01 0.343D-01-0.702D-01-0.110D+00-0.124D+00

Coeff-Com: 0.267D+00 0.980D+00

Coeff: 0.849D-05-0.170D-06-0.149D-03-0.276D-03-0.416D-03 0.711D-03

Coeff: 0.661D-02 0.170D-01 0.343D-01-0.702D-01-0.110D+00-0.124D+00

Coeff: 0.267D+00 0.980D+00

Gap= 0.093 Goal= None Shift= 0.000

Gap= 0.058 Goal= None Shift= 0.000

RMSDP=2.87D-08 MaxDP=1.09D-06 DE=-1.12D-09 OVMax= 1.07D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 1.17D-08 CP: 9.95D-01 1.56D-01 1.03D+00 6.81D-01 7.19D-01

CP: 7.28D-01 8.38D-01 1.19D+00 1.78D+00 1.95D+00

CP: 1.39D+00 1.57D+00 1.56D+00 1.17D+00

E= -1914.20081549129 Delta-E= -0.000000000426 Rises=F Damp=F

DIIS: error= 4.47D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1914.20081549129 IErMin=15 ErrMin= 4.47D-07

ErrMax= 4.47D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.22D-10 BMatP= 2.82D-10

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

Coeff-Com: 0.382D-05 0.121D-05-0.505D-04-0.136D-03-0.361D-03-0.270D-03

Coeff-Com: 0.181D-02 0.606D-02 0.191D-01-0.164D-01-0.492D-01-0.157D+00

Coeff-Com: 0.193D-01 0.591D+00 0.586D+00

Coeff: 0.382D-05 0.121D-05-0.505D-04-0.136D-03-0.361D-03-0.270D-03

Coeff: 0.181D-02 0.606D-02 0.191D-01-0.164D-01-0.492D-01-0.157D+00

Coeff: 0.193D-01 0.591D+00 0.586D+00

Gap= 0.093 Goal= None Shift= 0.000

Gap= 0.058 Goal= None Shift= 0.000

RMSDP=9.86D-09 MaxDP=4.32D-07 DE=-4.26D-10 OVMax= 3.60D-06

Error on total polarization charges = 0.07928

SCF Done: E(UB3LYP) = -1914.20081549 A.U. after 15 cycles

NFock= 15 Conv=0.99D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7873 S= 0.5185

<L.S>= 0.000000000000E+00

KE= 1.906169451820D+03 PE=-1.516218132552D+04 EE= 5.968062932893D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.42

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7873, after 0.7512

Leave Link 502 at Sun Aug 18 14:13:16 2019, MaxMem= 2013265920 cpu: 2827.1

(Enter /home/kira/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

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

GePol: Maximum number of non-zero 1st derivatives = 186

Leave Link 701 at Sun Aug 18 14:13:34 2019, MaxMem= 2013265920 cpu: 140.6

(Enter /home/kira/g09/l702.exe)

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

Leave Link 702 at Sun Aug 18 14:13:34 2019, MaxMem= 2013265920 cpu: 0.2

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

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

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

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Sun Aug 18 14:14:12 2019, MaxMem= 2013265920 cpu: 302.8

(Enter /home/kira/g09/l716.exe)

Dipole =-6.14878923D-13-6.25277607D-13-2.67078005D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.004416289 0.001270536 0.000359188

2 6 -0.005667935 -0.001688091 0.000600195

3 7 0.000000000 -0.000991559 -0.001217859

4 6 0.005667935 -0.001688091 0.000600195

5 6 -0.004416289 0.001270536 0.000359188

6 6 -0.002929319 0.000792140 -0.000173301

7 6 -0.001656229 -0.000500850 -0.000727832

8 7 0.001172475 -0.000000000 0.000775243

9 6 -0.001656229 0.000500850 -0.000727832

10 6 0.000621283 0.000607476 0.000019144

11 6 0.000621283 -0.000607476 0.000019144

12 6 0.002929319 0.000792140 -0.000173301

13 6 0.001656229 -0.000500850 -0.000727832

14 6 -0.000621283 -0.000607476 0.000019144

15 6 -0.000621283 0.000607476 0.000019144

16 6 0.001656229 0.000500850 -0.000727832

17 7 -0.001172475 0.000000000 0.000775243

18 6 0.002929319 -0.000792140 -0.000173301

19 6 -0.005667935 0.001688091 0.000600195

20 6 0.004416289 -0.001270536 0.000359188

21 6 -0.004416289 -0.001270536 0.000359188

22 6 0.005667935 0.001688091 0.000600195

23 7 -0.000000000 0.000991559 -0.001217859

24 6 -0.002929319 -0.000792140 -0.000173301

25 6 -0.000102270 -0.000408771 0.000213128

26 6 0.000715291 -0.000338752 0.000374498

27 6 -0.000341567 -0.000053493 -0.000261080

28 6 0.000147072 0.000155164 0.000026547

29 6 -0.000042213 -0.000331178 0.000255664

30 6 -0.000284459 0.000882295 -0.000381752

31 6 -0.000147072 0.000155164 0.000026547

32 6 0.000341567 -0.000053493 -0.000261080

33 6 -0.000715291 -0.000338752 0.000374498

34 6 0.000102270 -0.000408771 0.000213128

35 6 0.000284459 0.000882295 -0.000381752

36 6 0.000042213 -0.000331178 0.000255664

37 6 -0.000102270 0.000408771 0.000213128

38 6 -0.000284459 -0.000882295 -0.000381752

39 6 -0.000042213 0.000331178 0.000255664

40 6 0.000147072 -0.000155164 0.000026547

41 6 -0.000341567 0.000053493 -0.000261080

42 6 0.000715291 0.000338752 0.000374498

43 6 0.000102270 0.000408771 0.000213128

44 6 0.000284459 -0.000882295 -0.000381752

45 6 0.000042213 0.000331178 0.000255664

46 6 -0.000147072 -0.000155164 0.000026547

47 6 0.000341567 0.000053493 -0.000261080

48 6 -0.000715291 0.000338752 0.000374498

49 1 -0.000411655 0.000198020 -0.000180581

50 1 0.000411655 0.000198020 -0.000180581

51 1 0.000171034 -0.000254757 0.000072068

52 1 0.000171034 0.000254757 0.000072068

53 1 -0.000171034 0.000254757 0.000072068

54 1 -0.000171034 -0.000254757 0.000072068

55 1 -0.000411655 -0.000198020 -0.000180581

56 1 0.000411655 -0.000198020 -0.000180581

57 1 0.000021565 0.000160919 -0.000274754

58 1 -0.000136032 -0.000002220 0.000074721

59 1 -0.000003622 -0.000003614 -0.000005438

60 1 0.000004093 -0.000138024 -0.000082694

61 1 0.000132317 0.000028089 0.000280585

62 1 0.000003622 -0.000003614 -0.000005438

63 1 0.000136032 -0.000002220 0.000074721

64 1 -0.000021565 0.000160919 -0.000274754

65 1 -0.000132317 0.000028089 0.000280585

66 1 -0.000004093 -0.000138024 -0.000082694

67 1 0.000132317 -0.000028089 0.000280585

68 1 0.000004093 0.000138024 -0.000082694

69 1 -0.000003622 0.000003614 -0.000005438

70 1 -0.000136032 0.000002220 0.000074721

71 1 0.000021565 -0.000160919 -0.000274754

72 1 -0.000132317 -0.000028089 0.000280585

73 1 -0.000004093 0.000138024 -0.000082694

74 1 0.000003622 0.000003614 -0.000005438

75 1 0.000136032 0.000002220 0.000074721

76 1 -0.000021565 -0.000160919 -0.000274754

77 1 0.000000000 0.000598723 0.000066002

78 1 -0.000000000 -0.000598723 0.000066002

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

Cartesian Forces: Max 0.005667935 RMS 0.001136026

Leave Link 716 at Sun Aug 18 14:14:12 2019, MaxMem= 2013265920 cpu: 0.2

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

Internal Forces: Max 0.003023486 RMS 0.000459103

Search for a local minimum.

Step number 5 out of a maximum of 452

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

RMS Force = .45910D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 4 5

DE= 7.25D-05 DEPred=-3.92D-04 R=-1.85D-01

Trust test=-1.85D-01 RLast= 4.76D-01 DXMaxT set to 4.74D-01

ITU= -1 1 1 1 0

Eigenvalues --- 0.00560 0.00861 0.00861 0.00861 0.01491

Eigenvalues --- 0.01653 0.01669 0.01672 0.01678 0.01682

Eigenvalues --- 0.01697 0.01710 0.01710 0.01710 0.01714

Eigenvalues --- 0.01732 0.01754 0.01831 0.01857 0.01869

Eigenvalues --- 0.01883 0.01907 0.01909 0.01911 0.01918

Eigenvalues --- 0.01952 0.02007 0.02014 0.02017 0.02022

Eigenvalues --- 0.02026 0.02034 0.02042 0.02059 0.02068

Eigenvalues --- 0.02087 0.02099 0.02099 0.02099 0.02099

Eigenvalues --- 0.02107 0.02129 0.02133 0.02133 0.02133

Eigenvalues --- 0.02142 0.02142 0.02142 0.02142 0.02161

Eigenvalues --- 0.02161 0.02161 0.02165 0.02165 0.02165

Eigenvalues --- 0.02165 0.02171 0.02171 0.02171 0.02171

Eigenvalues --- 0.02175 0.02175 0.02175 0.02176 0.02176

Eigenvalues --- 0.02176 0.02176 0.02178 0.02193 0.02211

Eigenvalues --- 0.02218 0.02224 0.02235 0.02464 0.03369

Eigenvalues --- 0.15980 0.15980 0.15982 0.15982 0.15989

Eigenvalues --- 0.15990 0.15991 0.15991 0.15991 0.15991

Eigenvalues --- 0.15993 0.15993 0.15993 0.15993 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 0.16007 0.16032 0.16175

Eigenvalues --- 0.21998 0.21998 0.21998 0.22001 0.22001

Eigenvalues --- 0.22001 0.22001 0.22010 0.22654 0.22781

Eigenvalues --- 0.22788 0.22791 0.23341 0.23474 0.23474

Eigenvalues --- 0.23474 0.23523 0.23584 0.24085 0.24635

Eigenvalues --- 0.24637 0.24752 0.24995 0.24995 0.24995

Eigenvalues --- 0.24998 0.24999 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25006 0.25296

Eigenvalues --- 0.25984 0.27869 0.33146 0.33146 0.33146

Eigenvalues --- 0.33344 0.34567 0.34596 0.35400 0.35400

Eigenvalues --- 0.35400 0.35400 0.35400 0.35400 0.35400

Eigenvalues --- 0.35405 0.35405 0.35405 0.35405 0.35424

Eigenvalues --- 0.35452 0.35452 0.35452 0.35457 0.35461

Eigenvalues --- 0.35461 0.35461 0.35531 0.36108 0.36108

Eigenvalues --- 0.36108 0.36146 0.36232 0.36232 0.36232

Eigenvalues --- 0.36282 0.36871 0.37054 0.37369 0.37395

Eigenvalues --- 0.39528 0.39922 0.41996 0.41996 0.41996

Eigenvalues --- 0.42164 0.42165 0.42165 0.42165 0.42192

Eigenvalues --- 0.43228 0.43468 0.44364 0.44410 0.44720

Eigenvalues --- 0.45285 0.45366 0.45487 0.45530 0.45632

Eigenvalues --- 0.45849 0.45856 0.45856 0.45856 0.45882

Eigenvalues --- 0.46150 0.46150 0.46150 0.46259 0.46278

Eigenvalues --- 0.46645 0.46645 0.46645 0.46645 0.46834

Eigenvalues --- 0.46834 0.46834 0.46948 0.47534 0.48555

Eigenvalues --- 0.48616 0.49719 0.49847 0.50637 0.51845

Eigenvalues --- 0.53068 0.53762 0.60257

En-DIIS/RFO-DIIS IScMMF= 0 using points: 5 4 3 2

RFO step: Lambda=-1.70436024D-04.

NNeg= 0 NP= 4 Switch= 2.50D-03 Rises=F DC= 4.52D-04 SmlDif= 1.00D-05

RMS Error= 0.1210077793D-02 NUsed= 4 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.60723 -0.19464 0.31510 0.27231

Iteration 1 RMS(Cart)= 0.11282748 RMS(Int)= 0.00323894

Iteration 2 RMS(Cart)= 0.00662092 RMS(Int)= 0.00034848

Iteration 3 RMS(Cart)= 0.00002249 RMS(Int)= 0.00034840

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00034840

ITry= 1 IFail=0 DXMaxC= 3.87D-01 DCOld= 1.00D+10 DXMaxT= 4.74D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 9.36D-09 for atom 69.

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

(Linear) (Quad) (Total)

R1 2.68784 0.00188 0.00503 0.00077 0.00566 2.69350

R2 2.60573 -0.00238 -0.00738 -0.00021 -0.00807 2.59766

R3 2.03520 0.00035 0.00044 0.00036 0.00080 2.03600

R4 2.58710 0.00097 0.00181 0.00083 0.00303 2.59013

R5 2.68228 -0.00302 -0.00752 -0.00134 -0.00887 2.67342

R6 2.58710 0.00097 0.00181 0.00083 0.00303 2.59013

R7 1.90990 -0.00060 0.00214 -0.00147 0.00066 1.91057

R8 2.68784 0.00188 0.00503 0.00077 0.00566 2.69350

R9 2.68228 -0.00302 -0.00752 -0.00134 -0.00887 2.67342

R10 2.03520 0.00035 0.00044 0.00036 0.00080 2.03600

R11 2.66637 0.00027 -0.00171 0.00089 -0.00082 2.66555

R12 2.79399 0.00004 0.00575 -0.00094 0.00481 2.79880

R13 2.58304 -0.00044 -0.00139 0.00031 -0.00068 2.58236

R14 2.74708 0.00071 0.00223 0.00025 0.00234 2.74942

R15 2.58304 -0.00044 -0.00139 0.00031 -0.00068 2.58236

R16 2.74708 0.00071 0.00223 0.00025 0.00234 2.74942

R17 2.66637 0.00027 -0.00171 0.00089 -0.00082 2.66555

R18 2.56363 -0.00033 -0.00203 0.00057 -0.00196 2.56167

R19 2.03767 0.00026 0.00001 0.00041 0.00042 2.03809

R20 2.03767 0.00026 0.00001 0.00041 0.00042 2.03809

R21 2.66637 0.00027 -0.00171 0.00089 -0.00082 2.66555

R22 2.79399 0.00004 0.00575 -0.00094 0.00481 2.79880

R23 2.74708 0.00071 0.00223 0.00025 0.00234 2.74942

R24 2.58304 -0.00044 -0.00139 0.00031 -0.00068 2.58236

R25 2.56363 -0.00033 -0.00203 0.00057 -0.00196 2.56167

R26 2.03767 0.00026 0.00001 0.00041 0.00042 2.03809

R27 2.74708 0.00071 0.00223 0.00025 0.00234 2.74942

R28 2.03767 0.00026 0.00001 0.00041 0.00042 2.03809

R29 2.58304 -0.00044 -0.00139 0.00031 -0.00068 2.58236

R30 2.66637 0.00027 -0.00171 0.00089 -0.00082 2.66555

R31 2.68228 -0.00302 -0.00752 -0.00134 -0.00887 2.67342

R32 2.79399 0.00004 0.00575 -0.00094 0.00481 2.79880

R33 2.68784 0.00188 0.00503 0.00077 0.00566 2.69350

R34 2.58710 0.00097 0.00181 0.00083 0.00303 2.59013

R35 2.60573 -0.00238 -0.00738 -0.00021 -0.00807 2.59766

R36 2.03520 0.00035 0.00044 0.00036 0.00080 2.03600

R37 2.68784 0.00188 0.00503 0.00077 0.00566 2.69350

R38 2.03520 0.00035 0.00044 0.00036 0.00080 2.03600

R39 2.58710 0.00097 0.00181 0.00083 0.00303 2.59013

R40 2.68228 -0.00302 -0.00752 -0.00134 -0.00887 2.67342

R41 1.90990 -0.00060 0.00214 -0.00147 0.00066 1.91057

R42 2.79399 0.00004 0.00575 -0.00094 0.00481 2.79880

R43 2.65351 -0.00017 -0.00322 0.00068 -0.00254 2.65097

R44 2.65364 -0.00015 -0.00326 0.00074 -0.00252 2.65112

R45 2.62798 -0.00027 0.00049 -0.00017 0.00032 2.62830

R46 2.04710 0.00017 0.00085 -0.00010 0.00074 2.04785

R47 2.63483 0.00012 0.00013 0.00005 0.00018 2.63501

R48 2.04950 -0.00004 -0.00006 -0.00000 -0.00006 2.04944

R49 2.63537 0.00011 0.00010 0.00002 0.00012 2.63549

R50 2.04978 -0.00001 -0.00006 0.00004 -0.00002 2.04977

R51 2.62749 -0.00026 0.00043 -0.00013 0.00030 2.62779

R52 2.04952 -0.00004 -0.00007 -0.00000 -0.00007 2.04945

R53 2.04692 0.00016 0.00086 -0.00008 0.00078 2.04769

R54 2.63483 0.00012 0.00013 0.00005 0.00018 2.63501

R55 2.63537 0.00011 0.00010 0.00002 0.00012 2.63549

R56 2.04978 -0.00001 -0.00006 0.00004 -0.00002 2.04977

R57 2.62798 -0.00027 0.00049 -0.00017 0.00032 2.62830

R58 2.04950 -0.00004 -0.00006 -0.00000 -0.00006 2.04944

R59 2.65351 -0.00017 -0.00322 0.00068 -0.00254 2.65097

R60 2.04710 0.00017 0.00085 -0.00010 0.00074 2.04785

R61 2.65364 -0.00015 -0.00326 0.00074 -0.00252 2.65112

R62 2.62749 -0.00026 0.00043 -0.00013 0.00030 2.62779

R63 2.04692 0.00016 0.00086 -0.00008 0.00078 2.04769

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R66 2.65351 -0.00017 -0.00322 0.00068 -0.00254 2.65097

R67 2.62749 -0.00026 0.00043 -0.00013 0.00030 2.62779

R68 2.04692 0.00016 0.00086 -0.00008 0.00078 2.04769

R69 2.63537 0.00011 0.00010 0.00002 0.00012 2.63549

R70 2.04952 -0.00004 -0.00007 -0.00000 -0.00007 2.04945

R71 2.63483 0.00012 0.00013 0.00005 0.00018 2.63501

R72 2.04978 -0.00001 -0.00006 0.00004 -0.00002 2.04977

R73 2.62798 -0.00027 0.00049 -0.00017 0.00032 2.62830

R74 2.04950 -0.00004 -0.00006 -0.00000 -0.00006 2.04944

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R76 2.65364 -0.00015 -0.00326 0.00074 -0.00252 2.65112

R77 2.65351 -0.00017 -0.00322 0.00068 -0.00254 2.65097

R78 2.62749 -0.00026 0.00043 -0.00013 0.00030 2.62779

R79 2.04692 0.00016 0.00086 -0.00008 0.00078 2.04769

R80 2.63537 0.00011 0.00010 0.00002 0.00012 2.63549

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A1 1.88061 0.00061 0.00110 0.00086 0.00208 1.88269

A2 2.18737 -0.00055 -0.00247 -0.00078 -0.00329 2.18408

A3 2.21469 -0.00006 0.00153 -0.00011 0.00137 2.21606

A4 1.86906 -0.00070 -0.00029 -0.00176 -0.00199 1.86707

A5 2.21201 0.00105 -0.00204 0.00251 -0.00087 2.21114

A6 2.20200 -0.00035 0.00237 -0.00082 0.00290 2.20490

A7 1.92406 0.00020 -0.00112 0.00224 0.00074 1.92479

A8 2.17956 -0.00010 0.00051 -0.00111 -0.00039 2.17917

A9 2.17956 -0.00010 0.00051 -0.00111 -0.00039 2.17917

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A12 2.21201 0.00105 -0.00204 0.00251 -0.00087 2.21114

A13 1.88061 0.00061 0.00110 0.00086 0.00208 1.88269

A14 2.21469 -0.00006 0.00153 -0.00011 0.00137 2.21606

A15 2.18737 -0.00055 -0.00247 -0.00078 -0.00329 2.18408

A16 2.17609 0.00009 0.00709 -0.00137 0.00756 2.18365

A17 2.03920 -0.00010 -0.00267 0.00046 -0.00313 2.03607

A18 2.06789 0.00001 -0.00442 0.00091 -0.00443 2.06346

A19 2.17844 0.00048 0.00400 0.00080 0.00618 2.18462

A20 2.17051 -0.00051 -0.00504 -0.00008 -0.00645 2.16407

A21 1.93405 0.00002 0.00109 -0.00090 0.00031 1.93435

A22 1.84160 0.00017 -0.00067 0.00166 0.00050 1.84210

A23 1.93405 0.00002 0.00109 -0.00090 0.00031 1.93435

A24 2.17844 0.00048 0.00400 0.00080 0.00618 2.18462

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A35 2.17051 -0.00051 -0.00504 -0.00008 -0.00645 2.16407

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A52 2.20200 -0.00035 0.00237 -0.00082 0.00290 2.20490

A53 1.86906 -0.00070 -0.00029 -0.00176 -0.00199 1.86707

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A55 2.18737 -0.00055 -0.00247 -0.00078 -0.00329 2.18408

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A58 2.21469 -0.00006 0.00153 -0.00011 0.00137 2.21606

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A64 2.17956 -0.00010 0.00051 -0.00111 -0.00039 2.17917

A65 2.17956 -0.00010 0.00051 -0.00111 -0.00039 2.17917

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A67 2.06789 0.00001 -0.00442 0.00091 -0.00443 2.06346

A68 2.03920 -0.00010 -0.00267 0.00046 -0.00313 2.03607

A69 2.10554 -0.00001 -0.00160 0.00072 -0.00088 2.10467

A70 2.09842 0.00040 -0.00099 0.00129 0.00030 2.09872

A71 2.07922 -0.00040 0.00260 -0.00201 0.00058 2.07980

A72 2.09942 0.00034 -0.00094 0.00117 0.00023 2.09965

A73 2.08647 0.00008 0.00114 -0.00004 0.00112 2.08758

A74 2.09682 -0.00042 -0.00007 -0.00119 -0.00125 2.09558

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A76 2.08952 -0.00008 -0.00082 0.00004 -0.00078 2.08874

A77 2.09638 0.00011 0.00103 -0.00014 0.00089 2.09727

A78 2.09338 -0.00020 -0.00030 -0.00049 -0.00078 2.09260

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A80 2.09484 0.00010 0.00018 0.00024 0.00042 2.09526

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A82 2.09625 0.00012 0.00107 -0.00015 0.00092 2.09718

A83 2.08959 -0.00007 -0.00086 0.00009 -0.00077 2.08882

A84 2.09943 0.00035 -0.00090 0.00119 0.00029 2.09972

A85 2.08582 0.00006 0.00114 -0.00011 0.00105 2.08687

A86 2.09749 -0.00040 -0.00010 -0.00116 -0.00125 2.09625

A87 2.09338 -0.00020 -0.00030 -0.00049 -0.00078 2.09260

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A89 2.09484 0.00010 0.00018 0.00024 0.00042 2.09526

A90 2.09728 -0.00003 -0.00021 0.00010 -0.00011 2.09717

A91 2.09638 0.00011 0.00103 -0.00014 0.00089 2.09727

A92 2.08952 -0.00008 -0.00082 0.00004 -0.00078 2.08874

A93 2.09942 0.00034 -0.00094 0.00117 0.00023 2.09965

A94 2.09682 -0.00042 -0.00007 -0.00119 -0.00125 2.09558

A95 2.08647 0.00008 0.00114 -0.00004 0.00112 2.08758

A96 2.10554 -0.00001 -0.00160 0.00072 -0.00088 2.10467

A97 2.09842 0.00040 -0.00099 0.00129 0.00030 2.09872

A98 2.07922 -0.00040 0.00260 -0.00201 0.00058 2.07980

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A103 2.09625 0.00012 0.00107 -0.00015 0.00092 2.09718

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A105 2.09842 0.00040 -0.00099 0.00129 0.00030 2.09872

A106 2.10554 -0.00001 -0.00160 0.00072 -0.00088 2.10467

A107 2.07922 -0.00040 0.00260 -0.00201 0.00058 2.07980

A108 2.09943 0.00035 -0.00090 0.00119 0.00029 2.09972

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A113 2.09625 0.00012 0.00107 -0.00015 0.00092 2.09718

A114 2.09338 -0.00020 -0.00030 -0.00049 -0.00078 2.09260

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A123 2.09842 0.00040 -0.00099 0.00129 0.00030 2.09872

A124 2.10554 -0.00001 -0.00160 0.00072 -0.00088 2.10467

A125 2.07922 -0.00040 0.00260 -0.00201 0.00058 2.07980

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A127 2.08582 0.00006 0.00114 -0.00011 0.00105 2.08687

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A129 2.09734 -0.00005 -0.00020 0.00005 -0.00015 2.09718

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A131 2.09625 0.00012 0.00107 -0.00015 0.00092 2.09718

A132 2.09338 -0.00020 -0.00030 -0.00049 -0.00078 2.09260

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A134 2.09496 0.00010 0.00012 0.00024 0.00036 2.09532

A135 2.09728 -0.00003 -0.00021 0.00010 -0.00011 2.09717

A136 2.09638 0.00011 0.00103 -0.00014 0.00089 2.09727

A137 2.08952 -0.00008 -0.00082 0.00004 -0.00078 2.08874

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A139 2.08647 0.00008 0.00114 -0.00004 0.00112 2.08758

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D2 -3.09703 -0.00003 -0.01622 0.00060 -0.01552 -3.11255

D3 -3.07958 -0.00027 -0.01448 -0.00368 -0.01816 -3.09774

D4 0.07715 -0.00009 -0.02271 0.00159 -0.02108 0.05607

D5 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D6 -3.10835 -0.00005 -0.00657 0.00102 -0.00558 -3.11393

D7 3.10835 0.00005 0.00657 -0.00102 0.00558 3.11393

D8 0.00000 0.00000 0.00000 0.00000 -0.00000 0.00000

D9 -0.04901 0.00035 0.01334 0.00771 0.02099 -0.02802

D10 3.09790 0.00012 0.00173 0.00277 0.00456 3.10246

D11 3.07755 0.00019 0.02153 0.00252 0.02386 3.10141

D12 -0.05873 -0.00005 0.00991 -0.00242 0.00743 -0.05130

D13 -2.94504 -0.00014 -0.04787 0.01015 -0.03769 -2.98273

D14 0.19635 -0.00024 -0.04925 0.00665 -0.04258 0.15377

D15 0.21448 0.00007 -0.05762 0.01639 -0.04112 0.17336

D16 -2.92731 -0.00003 -0.05900 0.01288 -0.04600 -2.97332

D17 0.04901 -0.00035 -0.01334 -0.00771 -0.02099 0.02802

D18 -3.07755 -0.00019 -0.02153 -0.00252 -0.02386 -3.10141

D19 -3.09790 -0.00012 -0.00173 -0.00277 -0.00456 -3.10246

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D23 3.09703 0.00003 0.01622 -0.00060 0.01552 3.11255

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D27 2.94504 0.00014 0.04787 -0.01015 0.03769 2.98273

D28 -0.19635 0.00024 0.04925 -0.00665 0.04258 -0.15377

D29 -0.20431 -0.00003 0.04881 -0.01296 0.03573 -0.16858

D30 2.95971 0.00021 0.03498 -0.00208 0.03289 2.99260

D31 2.93707 -0.00013 0.04742 -0.01652 0.03078 2.96785

D32 -0.18209 0.00011 0.03358 -0.00564 0.02794 -0.15416

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D36 -0.91595 -0.00035 -0.06920 -0.00147 -0.07068 -0.98663

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D63 -2.22432 0.00033 0.06835 0.00126 0.06961 -2.15471

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D89 -0.91595 -0.00035 -0.06920 -0.00147 -0.07068 -0.98663

D90 2.22432 -0.00033 -0.06835 -0.00126 -0.06961 2.15471

D91 2.22545 -0.00044 -0.07046 -0.00475 -0.07521 2.15024

D92 -0.91746 -0.00042 -0.06961 -0.00454 -0.07414 -0.99160

D93 3.09703 0.00003 0.01622 -0.00060 0.01552 3.11255

D94 -0.07715 0.00009 0.02271 -0.00159 0.02108 -0.05607

D95 -0.02942 0.00021 0.00800 0.00466 0.01260 -0.01682

D96 3.07958 0.00027 0.01448 0.00368 0.01816 3.09774

D97 -3.07755 -0.00019 -0.02153 -0.00252 -0.02386 -3.10141

D98 0.05873 0.00005 -0.00991 0.00242 -0.00743 0.05130

D99 0.04901 -0.00035 -0.01334 -0.00771 -0.02099 0.02802

D100 -3.09790 -0.00012 -0.00173 -0.00277 -0.00456 -3.10246

D101 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D102 3.10835 0.00005 0.00657 -0.00102 0.00558 3.11393

D103 -3.10835 -0.00005 -0.00657 0.00102 -0.00558 -3.11393

D104 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D105 0.02942 -0.00021 -0.00800 -0.00466 -0.01260 0.01682

D106 -3.09703 -0.00003 -0.01622 0.00060 -0.01552 -3.11255

D107 -3.07958 -0.00027 -0.01448 -0.00368 -0.01816 -3.09774

D108 0.07715 -0.00009 -0.02271 0.00159 -0.02108 0.05607

D109 -0.04901 0.00035 0.01334 0.00771 0.02099 -0.02802

D110 3.09790 0.00012 0.00173 0.00277 0.00456 3.10246

D111 3.07755 0.00019 0.02153 0.00252 0.02386 3.10141

D112 -0.05873 -0.00005 0.00991 -0.00242 0.00743 -0.05130

D113 -2.94504 -0.00014 -0.04787 0.01015 -0.03769 -2.98273

D114 0.19635 -0.00024 -0.04925 0.00665 -0.04258 0.15377

D115 0.21448 0.00007 -0.05762 0.01639 -0.04112 0.17336

D116 -2.92731 -0.00003 -0.05900 0.01288 -0.04600 -2.97332

D117 0.91595 0.00035 0.06920 0.00147 0.07068 0.98663

D118 -2.22432 0.00033 0.06835 0.00126 0.06961 -2.15471

D119 -2.22545 0.00044 0.07046 0.00475 0.07521 -2.15024

D120 0.91746 0.00042 0.06961 0.00454 0.07414 0.99160

D121 -3.12891 -0.00005 -0.00184 -0.00028 -0.00211 -3.13102

D122 -0.02051 -0.00006 0.00420 -0.00248 0.00171 -0.01879

D123 0.01138 -0.00002 -0.00100 -0.00007 -0.00106 0.01032

D124 3.11978 -0.00003 0.00504 -0.00227 0.00277 3.12255

D125 -3.13260 -0.00001 -0.00021 -0.00012 -0.00034 -3.13294

D126 -0.02300 -0.00003 0.00640 -0.00277 0.00363 -0.01937

D127 0.01029 -0.00004 -0.00105 -0.00033 -0.00138 0.00890

D128 3.11989 -0.00006 0.00556 -0.00298 0.00258 3.12247

D129 -0.02185 0.00006 0.00199 0.00029 0.00229 -0.01957

D130 3.11740 0.00006 0.00419 -0.00024 0.00396 3.12136

D131 -3.13005 0.00006 -0.00409 0.00249 -0.00160 -3.13165

D132 0.00920 0.00007 -0.00189 0.00196 0.00007 0.00927

D133 0.01061 -0.00003 -0.00094 -0.00013 -0.00107 0.00954

D134 -3.13063 -0.00004 -0.00115 -0.00015 -0.00130 -3.13193

D135 -3.12863 -0.00004 -0.00315 0.00040 -0.00275 -3.13138

D136 0.01331 -0.00004 -0.00336 0.00038 -0.00297 0.01034

D137 0.01110 -0.00004 -0.00111 -0.00029 -0.00139 0.00970

D138 -3.12804 -0.00004 -0.00357 0.00049 -0.00308 -3.13112

D139 -3.13085 -0.00004 -0.00090 -0.00027 -0.00117 -3.13202

D140 0.01320 -0.00004 -0.00336 0.00051 -0.00285 0.01035

D141 -0.02154 0.00007 0.00211 0.00051 0.00261 -0.01893

D142 -3.13093 0.00008 -0.00456 0.00315 -0.00142 -3.13235

D143 3.11760 0.00007 0.00456 -0.00027 0.00429 3.12190

D144 0.00821 0.00008 -0.00211 0.00237 0.00027 0.00848

D145 -0.01061 0.00003 0.00094 0.00013 0.00107 -0.00954

D146 3.12863 0.00004 0.00315 -0.00040 0.00275 3.13138

D147 3.13063 0.00004 0.00115 0.00015 0.00130 3.13193

D148 -0.01331 0.00004 0.00336 -0.00038 0.00297 -0.01034

D149 -0.01110 0.00004 0.00111 0.00029 0.00139 -0.00970

D150 3.12804 0.00004 0.00357 -0.00049 0.00308 3.13112

D151 3.13085 0.00004 0.00090 0.00027 0.00117 3.13202

D152 -0.01320 0.00004 0.00336 -0.00051 0.00285 -0.01035

D153 0.02185 -0.00006 -0.00199 -0.00029 -0.00229 0.01957

D154 3.13005 -0.00006 0.00409 -0.00249 0.00160 3.13165

D155 -3.11740 -0.00006 -0.00419 0.00024 -0.00396 -3.12136

D156 -0.00920 -0.00007 0.00189 -0.00196 -0.00007 -0.00927

D157 3.12891 0.00005 0.00184 0.00028 0.00211 3.13102

D158 -0.01138 0.00002 0.00100 0.00007 0.00106 -0.01032

D159 0.02051 0.00006 -0.00420 0.00248 -0.00171 0.01879

D160 -3.11978 0.00003 -0.00504 0.00227 -0.00277 -3.12255

D161 3.13260 0.00001 0.00021 0.00012 0.00034 3.13294

D162 0.02300 0.00003 -0.00640 0.00277 -0.00363 0.01937

D163 -0.01029 0.00004 0.00105 0.00033 0.00138 -0.00890

D164 -3.11989 0.00006 -0.00556 0.00298 -0.00258 -3.12247

D165 0.02154 -0.00007 -0.00211 -0.00051 -0.00261 0.01893

D166 -3.11760 -0.00007 -0.00456 0.00027 -0.00429 -3.12190

D167 3.13093 -0.00008 0.00456 -0.00315 0.00142 3.13235

D168 -0.00821 -0.00008 0.00211 -0.00237 -0.00027 -0.00848

D169 3.13260 0.00001 0.00021 0.00012 0.00034 3.13294

D170 0.02300 0.00003 -0.00640 0.00277 -0.00363 0.01937

D171 -0.01029 0.00004 0.00105 0.00033 0.00138 -0.00890

D172 -3.11989 0.00006 -0.00556 0.00298 -0.00258 -3.12247

D173 3.12891 0.00005 0.00184 0.00028 0.00211 3.13102

D174 0.02051 0.00006 -0.00420 0.00248 -0.00171 0.01879

D175 -0.01138 0.00002 0.00100 0.00007 0.00106 -0.01032

D176 -3.11978 0.00003 -0.00504 0.00227 -0.00277 -3.12255

D177 0.02154 -0.00007 -0.00211 -0.00051 -0.00261 0.01893

D178 -3.11760 -0.00007 -0.00456 0.00027 -0.00429 -3.12190

D179 3.13093 -0.00008 0.00456 -0.00315 0.00142 3.13235

D180 -0.00821 -0.00008 0.00211 -0.00237 -0.00027 -0.00848

D181 -0.01110 0.00004 0.00111 0.00029 0.00139 -0.00970

D182 3.13085 0.00004 0.00090 0.00027 0.00117 3.13202

D183 3.12804 0.00004 0.00357 -0.00049 0.00308 3.13112

D184 -0.01320 0.00004 0.00336 -0.00051 0.00285 -0.01035

D185 -0.01061 0.00003 0.00094 0.00013 0.00107 -0.00954

D186 3.12863 0.00004 0.00315 -0.00040 0.00275 3.13138

D187 3.13063 0.00004 0.00115 0.00015 0.00130 3.13193

D188 -0.01331 0.00004 0.00336 -0.00038 0.00297 -0.01034

D189 0.02185 -0.00006 -0.00199 -0.00029 -0.00229 0.01957

D190 3.13005 -0.00006 0.00409 -0.00249 0.00160 3.13165

D191 -3.11740 -0.00006 -0.00419 0.00024 -0.00396 -3.12136

D192 -0.00920 -0.00007 0.00189 -0.00196 -0.00007 -0.00927

D193 -3.13260 -0.00001 -0.00021 -0.00012 -0.00034 -3.13294

D194 -0.02300 -0.00003 0.00640 -0.00277 0.00363 -0.01937

D195 0.01029 -0.00004 -0.00105 -0.00033 -0.00138 0.00890

D196 3.11989 -0.00006 0.00556 -0.00298 0.00258 3.12247

D197 -3.12891 -0.00005 -0.00184 -0.00028 -0.00211 -3.13102

D198 -0.02051 -0.00006 0.00420 -0.00248 0.00171 -0.01879

D199 0.01138 -0.00002 -0.00100 -0.00007 -0.00106 0.01032

D200 3.11978 -0.00003 0.00504 -0.00227 0.00277 3.12255

D201 -0.02154 0.00007 0.00211 0.00051 0.00261 -0.01893

D202 3.11760 0.00007 0.00456 -0.00027 0.00429 3.12190

D203 -3.13093 0.00008 -0.00456 0.00315 -0.00142 -3.13235

D204 0.00821 0.00008 -0.00211 0.00237 0.00027 0.00848

D205 0.01110 -0.00004 -0.00111 -0.00029 -0.00139 0.00970

D206 -3.13085 -0.00004 -0.00090 -0.00027 -0.00117 -3.13202

D207 -3.12804 -0.00004 -0.00357 0.00049 -0.00308 -3.13112

D208 0.01320 -0.00004 -0.00336 0.00051 -0.00285 0.01035

D209 0.01061 -0.00003 -0.00094 -0.00013 -0.00107 0.00954

D210 -3.12863 -0.00004 -0.00315 0.00040 -0.00275 -3.13138

D211 -3.13063 -0.00004 -0.00115 -0.00015 -0.00130 -3.13193

D212 0.01331 -0.00004 -0.00336 0.00038 -0.00297 0.01034

D213 -0.02185 0.00006 0.00199 0.00029 0.00229 -0.01957

D214 -3.13005 0.00006 -0.00409 0.00249 -0.00160 -3.13165

D215 3.11740 0.00006 0.00419 -0.00024 0.00396 3.12136

D216 0.00920 0.00007 -0.00189 0.00196 0.00007 0.00927

Item Value Threshold Converged?

Maximum Force 0.003023 0.000450 NO

RMS Force 0.000459 0.000300 NO

Maximum Displacement 0.387188 0.001800 NO

RMS Displacement 0.116201 0.001200 NO

Predicted change in Energy=-2.499011D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Aug 18 14:14:12 2019, MaxMem= 2013265920 cpu: 1.5

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

Stoichiometry C44H30N4(1+,2)

Framework group C2V[SGV(H2N2),SGV'(N2),X(C44H28)]

Deg. of freedom 59

Full point group C2V NOp 4

RotChk: IX=0 Diff= 1.85D-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 -0.687312 4.184710 0.454032

2 6 0 -1.124698 2.867212 0.130807

3 7 0 0.000000 2.101425 -0.034360

4 6 0 1.124698 2.867212 0.130807

5 6 0 0.687312 4.184710 0.454032

6 6 0 2.463330 2.431711 -0.009954

7 6 0 2.868849 1.088078 -0.150831

8 7 0 2.058601 -0.000000 0.013405

9 6 0 2.868849 -1.088078 -0.150831

10 6 0 4.227438 -0.677789 -0.471330

11 6 0 4.227438 0.677789 -0.471330

12 6 0 -2.463330 2.431711 -0.009954

13 6 0 -2.868849 1.088078 -0.150831

14 6 0 -4.227438 0.677789 -0.471330

15 6 0 -4.227438 -0.677789 -0.471330

16 6 0 -2.868849 -1.088078 -0.150831

17 7 0 -2.058601 0.000000 0.013405

18 6 0 -2.463330 -2.431711 -0.009954

19 6 0 -1.124698 -2.867212 0.130807

20 6 0 -0.687312 -4.184710 0.454032

21 6 0 0.687312 -4.184710 0.454032

22 6 0 1.124698 -2.867212 0.130807

23 7 0 -0.000000 -2.101425 -0.034360

24 6 0 2.463330 -2.431711 -0.009954

25 6 0 3.508111 3.481413 -0.000380

26 6 0 3.468442 4.536523 -0.924017

27 6 0 4.459603 5.512220 -0.917810

28 6 0 5.487597 5.460565 0.022871

29 6 0 5.527853 4.421509 0.952264

30 6 0 4.551986 3.431011 0.935541

31 6 0 -5.487597 5.460565 0.022871

32 6 0 -4.459603 5.512220 -0.917810

33 6 0 -3.468442 4.536523 -0.924017

34 6 0 -3.508111 3.481413 -0.000380

35 6 0 -4.551986 3.431011 0.935541

36 6 0 -5.527853 4.421509 0.952264

37 6 0 3.508111 -3.481413 -0.000380

38 6 0 4.551986 -3.431011 0.935541

39 6 0 5.527853 -4.421509 0.952264

40 6 0 5.487597 -5.460565 0.022871

41 6 0 4.459603 -5.512220 -0.917810

42 6 0 3.468442 -4.536523 -0.924017

43 6 0 -3.508111 -3.481413 -0.000380

44 6 0 -4.551986 -3.431011 0.935541

45 6 0 -5.527853 -4.421509 0.952264

46 6 0 -5.487597 -5.460565 0.022871

47 6 0 -4.459603 -5.512220 -0.917810

48 6 0 -3.468442 -4.536523 -0.924017

49 1 0 -1.335275 5.014711 0.682177

50 1 0 1.335275 5.014711 0.682177

51 1 0 5.053269 -1.334785 -0.693921

52 1 0 5.053269 1.334785 -0.693921

53 1 0 -5.053269 1.334785 -0.693921

54 1 0 -5.053269 -1.334785 -0.693921

55 1 0 -1.335275 -5.014711 0.682177

56 1 0 1.335275 -5.014711 0.682177

57 1 0 2.675328 4.572939 -1.661576

58 1 0 4.429337 6.313008 -1.648562

59 1 0 6.254719 6.227374 0.031872

60 1 0 6.319999 4.382502 1.691974

61 1 0 4.579239 2.628796 1.663470

62 1 0 -6.254719 6.227374 0.031872

63 1 0 -4.429337 6.313008 -1.648562

64 1 0 -2.675328 4.572939 -1.661576

65 1 0 -4.579239 2.628796 1.663470

66 1 0 -6.319999 4.382502 1.691974

67 1 0 4.579239 -2.628796 1.663470

68 1 0 6.319999 -4.382502 1.691974

69 1 0 6.254719 -6.227374 0.031872

70 1 0 4.429337 -6.313008 -1.648562

71 1 0 2.675328 -4.572939 -1.661576

72 1 0 -4.579239 -2.628796 1.663470

73 1 0 -6.319999 -4.382502 1.691974

74 1 0 -6.254719 -6.227374 0.031872

75 1 0 -4.429337 -6.313008 -1.648562

76 1 0 -2.675328 -4.572939 -1.661576

77 1 0 0.000000 1.111219 -0.238493

78 1 0 -0.000000 -1.111219 -0.238493

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

Rotational constants (GHZ): 0.0591767 0.0585244 0.0302639

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

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

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

There are 261 symmetry adapted cartesian basis functions of A1 symmetry.

There are 240 symmetry adapted cartesian basis functions of A2 symmetry.

There are 249 symmetry adapted cartesian basis functions of B1 symmetry.

There are 252 symmetry adapted cartesian basis functions of B2 symmetry.

There are 248 symmetry adapted basis functions of A1 symmetry.

There are 229 symmetry adapted basis functions of A2 symmetry.

There are 237 symmetry adapted basis functions of B1 symmetry.

There are 240 symmetry adapted basis functions of B2 symmetry.

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

161 alpha electrons 160 beta electrons

nuclear repulsion energy 5369.5179867404 Hartrees.

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

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

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

NAtoms= 78 NActive= 78 NUniq= 21 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=T Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2126783906 Hartrees.

Nuclear repulsion after empirical dispersion term = 5369.3053083498 Hartrees.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 78

GePol: Total number of spheres = 78

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

GePol: Number of points = 5790

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.14D-08

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 328

GePol: Fraction of low-weight points (<1% of avg) = 5.66%

GePol: Cavity surface area = 609.192 Ang\*\*2

GePol: Cavity volume = 626.174 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0021828543 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5369.3031254955 Hartrees.

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(Enter /home/kira/g09/l302.exe)

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

NBasis= 954 RedAO= T EigKep= 6.39D-05 NBF= 248 229 237 240

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 248 229 237 240

Precomputing XC quadrature grid using

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

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

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

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

DipDrv: MaxL=1.

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

Initial guess from the checkpoint file: "TPPcation.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) (B1) (A1) (B2) (A2) (A1) (B1) (A2) (B2)

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

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

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

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

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

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

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

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(A1)

Virtual (A1) (A1) (A1) (A1) (A1) (A1) (A1) (A1) (A1) (A1)

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The electronic state of the initial guess is 2-A1.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7873 S= 0.5185

Generating alternative initial guess.

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -1914.09119529754

Leave Link 401 at Sun Aug 18 14:14:20 2019, MaxMem= 2013265920 cpu: 46.5

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3049894 IEndB= 3049894 NGot= 2013265920 MDV= 2011237673

LenX= 2011237673 LenY= 2010232667

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

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

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

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

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

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 100572300.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.55D-15 for 5779.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.55D-15 for 4958 4849.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.11D-15 for 5779.

Iteration 1 A^-1\*A deviation from orthogonality is 4.23D-11 for 5207 5195.

E= -1914.09632823010

DIIS: error= 1.23D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.09632823010 IErMin= 1 ErrMin= 1.23D-02

ErrMax= 1.23D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.92D-01 BMatP= 1.92D-01

IDIUse=3 WtCom= 8.77D-01 WtEn= 1.23D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Recover alternate guess density for next cycle.

RMSDP=1.04D-03 MaxDP=5.29D-02 OVMax= 0.00D+00

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.04D-03 CP: 9.95D-01

E= -1913.31166414289 Delta-E= 0.784664087218 Rises=F Damp=F

Switch densities from cycles 1 and 2 for lowest energy.

DIIS: error= 4.61D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 1 EnMin= -1914.09632823010 IErMin= 1 ErrMin= 1.23D-02

ErrMax= 4.61D-02 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.80D+00 BMatP= 1.92D-01

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

Coeff-Com: 0.951D+00 0.487D-01

Coeff: 0.951D+00 0.487D-01

Gap= 0.499 Goal= None Shift= 0.000

Gap= 0.511 Goal= None Shift= 0.000

RMSDP=5.35D-03 MaxDP=3.32D-01 DE= 7.85D-01 OVMax= 5.51D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.00D-04 CP: 9.99D-01 6.07D-02

E= -1914.19756697195 Delta-E= -0.885902829066 Rises=F Damp=F

DIIS: error= 1.56D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.19756697195 IErMin= 3 ErrMin= 1.56D-03

ErrMax= 1.56D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 9.94D-03 BMatP= 1.92D-01

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

Coeff-Com: -0.535D-01 0.391D-01 0.101D+01

Coeff: -0.535D-01 0.391D-01 0.101D+01

Gap= 0.096 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=8.08D-05 MaxDP=3.62D-03 DE=-8.86D-01 OVMax= 1.59D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 6.51D-05 CP: 9.98D-01 1.06D-01 1.02D+00

E= -1914.20041966661 Delta-E= -0.002852694662 Rises=F Damp=F

DIIS: error= 1.10D-03 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.20041966661 IErMin= 4 ErrMin= 1.10D-03

ErrMax= 1.10D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.69D-03 BMatP= 9.94D-03

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

Coeff-Com: -0.327D-01 0.105D-01 0.441D+00 0.581D+00

Coeff: -0.327D-01 0.105D-01 0.441D+00 0.581D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.055 Goal= None Shift= 0.000

RMSDP=3.30D-05 MaxDP=2.21D-03 DE=-2.85D-03 OVMax= 7.32D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.45D-05 CP: 9.99D-01 1.02D-01 1.05D+00 6.86D-01

E= -1914.20100305379 Delta-E= -0.000583387175 Rises=F Damp=F

DIIS: error= 3.85D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.20100305379 IErMin= 5 ErrMin= 3.85D-04

ErrMax= 3.85D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 4.24D-04 BMatP= 2.69D-03

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

Coeff-Com: -0.103D-01 0.725D-03 0.107D+00 0.319D+00 0.584D+00

Coeff: -0.103D-01 0.725D-03 0.107D+00 0.319D+00 0.584D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=1.19D-05 MaxDP=8.92D-04 DE=-5.83D-04 OVMax= 3.24D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 7.24D-06 CP: 9.98D-01 1.02D-01 1.05D+00 7.46D-01 6.59D-01

E= -1914.20111454562 Delta-E= -0.000111491833 Rises=F Damp=F

DIIS: error= 6.78D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.20111454562 IErMin= 6 ErrMin= 6.78D-05

ErrMax= 6.78D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.09D-05 BMatP= 4.24D-04

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

Coeff-Com: -0.192D-02-0.422D-03 0.999D-02 0.848D-01 0.246D+00 0.662D+00

Coeff: -0.192D-02-0.422D-03 0.999D-02 0.848D-01 0.246D+00 0.662D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=3.03D-06 MaxDP=2.18D-04 DE=-1.11D-04 OVMax= 9.45D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.38D-06 CP: 9.98D-01 1.02D-01 1.05D+00 7.61D-01 7.00D-01

CP: 8.28D-01

E= -1914.20111927366 Delta-E= -0.000004728036 Rises=F Damp=F

DIIS: error= 3.92D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.20111927366 IErMin= 7 ErrMin= 3.92D-05

ErrMax= 3.92D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 5.35D-06 BMatP= 2.09D-05

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

Coeff-Com: 0.261D-03-0.328D-03-0.927D-02 0.330D-02 0.612D-01 0.374D+00

Coeff-Com: 0.570D+00

Coeff: 0.261D-03-0.328D-03-0.927D-02 0.330D-02 0.612D-01 0.374D+00

Coeff: 0.570D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=1.30D-06 MaxDP=8.87D-05 DE=-4.73D-06 OVMax= 3.81D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 9.62D-07 CP: 9.98D-01 1.02D-01 1.05D+00 7.63D-01 7.15D-01

CP: 8.95D-01 7.42D-01

E= -1914.20112080660 Delta-E= -0.000001532937 Rises=F Damp=F

DIIS: error= 1.46D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.20112080660 IErMin= 8 ErrMin= 1.46D-05

ErrMax= 1.46D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 4.28D-07 BMatP= 5.35D-06

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

Coeff-Com: 0.304D-03-0.894D-04-0.476D-02-0.766D-02-0.373D-03 0.826D-01

Coeff-Com: 0.226D+00 0.704D+00

Coeff: 0.304D-03-0.894D-04-0.476D-02-0.766D-02-0.373D-03 0.826D-01

Coeff: 0.226D+00 0.704D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=6.47D-07 MaxDP=7.54D-05 DE=-1.53D-06 OVMax= 3.49D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 5.53D-07 CP: 9.98D-01 1.02D-01 1.05D+00 7.65D-01 7.20D-01

CP: 9.02D-01 8.47D-01 1.08D+00

E= -1914.20112103461 Delta-E= -0.000000228013 Rises=F Damp=F

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

NSaved= 9 IEnMin= 9 EnMin= -1914.20112103461 IErMin= 8 ErrMin= 1.46D-05

ErrMax= 1.55D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.45D-07 BMatP= 4.28D-07

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

Coeff-Com: 0.114D-03 0.543D-04-0.165D-03-0.590D-02-0.192D-01-0.639D-01

Coeff-Com: -0.354D-01 0.460D+00 0.664D+00

Coeff: 0.114D-03 0.543D-04-0.165D-03-0.590D-02-0.192D-01-0.639D-01

Coeff: -0.354D-01 0.460D+00 0.664D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=4.96D-07 MaxDP=5.60D-05 DE=-2.28D-07 OVMax= 1.69D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 2.63D-07 CP: 9.98D-01 1.02D-01 1.05D+00 7.64D-01 7.23D-01

CP: 9.27D-01 8.92D-01 1.43D+00 8.61D-01

E= -1914.20112117219 Delta-E= -0.000000137583 Rises=F Damp=F

DIIS: error= 6.57D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.20112117219 IErMin=10 ErrMin= 6.57D-06

ErrMax= 6.57D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 4.49D-08 BMatP= 2.45D-07

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

Coeff-Com: -0.614D-04 0.513D-04 0.178D-02 0.302D-03-0.839D-02-0.595D-01

Coeff-Com: -0.104D+00-0.483D-01 0.293D+00 0.925D+00

Coeff: -0.614D-04 0.513D-04 0.178D-02 0.302D-03-0.839D-02-0.595D-01

Coeff: -0.104D+00-0.483D-01 0.293D+00 0.925D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=3.44D-07 MaxDP=4.37D-05 DE=-1.38D-07 OVMax= 2.11D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.51D-07 CP: 9.98D-01 1.02D-01 1.05D+00 7.65D-01 7.23D-01

CP: 9.34D-01 9.56D-01 1.62D+00 1.19D+00 1.01D+00

E= -1914.20112121596 Delta-E= -0.000000043773 Rises=F Damp=F

DIIS: error= 3.90D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.20112121596 IErMin=11 ErrMin= 3.90D-06

ErrMax= 3.90D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.54D-08 BMatP= 4.49D-08

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

Coeff-Com: -0.693D-04 0.169D-04 0.127D-02 0.171D-02-0.753D-03-0.239D-01

Coeff-Com: -0.619D-01-0.156D+00 0.988D-02 0.634D+00 0.596D+00

Coeff: -0.693D-04 0.169D-04 0.127D-02 0.171D-02-0.753D-03-0.239D-01

Coeff: -0.619D-01-0.156D+00 0.988D-02 0.634D+00 0.596D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=1.50D-07 MaxDP=1.75D-05 DE=-4.38D-08 OVMax= 5.62D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 5.85D-08 CP: 9.98D-01 1.02D-01 1.05D+00 7.64D-01 7.24D-01

CP: 9.39D-01 9.68D-01 1.72D+00 1.25D+00 1.30D+00

CP: 8.40D-01

E= -1914.20112122677 Delta-E= -0.000000010808 Rises=F Damp=F

DIIS: error= 8.96D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.20112122677 IErMin=12 ErrMin= 8.96D-07

ErrMax= 8.96D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 9.17D-10 BMatP= 2.54D-08

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

Coeff-Com: -0.134D-04-0.364D-05 0.160D-03 0.537D-03 0.920D-03 0.218D-03

Coeff-Com: -0.654D-02-0.421D-01-0.359D-01 0.910D-01 0.178D+00 0.814D+00

Coeff: -0.134D-04-0.364D-05 0.160D-03 0.537D-03 0.920D-03 0.218D-03

Coeff: -0.654D-02-0.421D-01-0.359D-01 0.910D-01 0.178D+00 0.814D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=3.47D-08 MaxDP=3.18D-06 DE=-1.08D-08 OVMax= 1.75D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 2.32D-08 CP: 9.98D-01 1.02D-01 1.05D+00 7.64D-01 7.24D-01

CP: 9.40D-01 9.69D-01 1.73D+00 1.27D+00 1.36D+00

CP: 9.16D-01 1.03D+00

E= -1914.20112122719 Delta-E= -0.000000000415 Rises=F Damp=F

DIIS: error= 3.57D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1914.20112122719 IErMin=13 ErrMin= 3.57D-07

ErrMax= 3.57D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.01D-10 BMatP= 9.17D-10

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

Coeff-Com: 0.424D-05-0.336D-05-0.124D-03-0.115D-04 0.529D-03 0.379D-02

Coeff-Com: 0.672D-02 0.685D-02-0.178D-01-0.556D-01-0.190D-01 0.363D+00

Coeff-Com: 0.712D+00

Coeff: 0.424D-05-0.336D-05-0.124D-03-0.115D-04 0.529D-03 0.379D-02

Coeff: 0.672D-02 0.685D-02-0.178D-01-0.556D-01-0.190D-01 0.363D+00

Coeff: 0.712D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=1.57D-08 MaxDP=8.36D-07 DE=-4.15D-10 OVMax= 6.85D-06

Cycle 14 Pass 1 IDiag 1:

RMSU= 1.07D-08 CP: 9.98D-01 1.02D-01 1.05D+00 7.64D-01 7.24D-01

CP: 9.40D-01 9.69D-01 1.73D+00 1.27D+00 1.37D+00

CP: 9.51D-01 1.17D+00 1.13D+00

E= -1914.20112122741 Delta-E= -0.000000000223 Rises=F Damp=F

DIIS: error= 2.35D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1914.20112122741 IErMin=14 ErrMin= 2.35D-07

ErrMax= 2.35D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 6.42D-11 BMatP= 3.01D-10

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

Coeff-Com: 0.541D-05 0.411D-06-0.900D-04-0.172D-03-0.152D-03 0.120D-02

Coeff-Com: 0.427D-02 0.161D-01 0.384D-02-0.460D-01-0.618D-01-0.110D+00

Coeff-Com: 0.249D+00 0.944D+00

Coeff: 0.541D-05 0.411D-06-0.900D-04-0.172D-03-0.152D-03 0.120D-02

Coeff: 0.427D-02 0.161D-01 0.384D-02-0.460D-01-0.618D-01-0.110D+00

Coeff: 0.249D+00 0.944D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=1.17D-08 MaxDP=5.78D-07 DE=-2.23D-10 OVMax= 4.90D-06

Cycle 15 Pass 1 IDiag 1:

RMSU= 5.61D-09 CP: 9.98D-01 1.02D-01 1.05D+00 7.64D-01 7.24D-01

CP: 9.40D-01 9.69D-01 1.73D+00 1.27D+00 1.38D+00

CP: 9.69D-01 1.27D+00 1.44D+00 1.20D+00

E= -1914.20112122748 Delta-E= -0.000000000071 Rises=F Damp=F

DIIS: error= 1.92D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1914.20112122748 IErMin=15 ErrMin= 1.92D-07

ErrMax= 1.92D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.49D-11 BMatP= 6.42D-11

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

Coeff-Com: 0.221D-05 0.753D-06-0.251D-04-0.907D-04-0.189D-03-0.589D-04

Coeff-Com: 0.100D-02 0.742D-02 0.497D-02-0.137D-01-0.300D-01-0.132D+00

Coeff-Com: -0.506D-02 0.511D+00 0.656D+00

Coeff: 0.221D-05 0.753D-06-0.251D-04-0.907D-04-0.189D-03-0.589D-04

Coeff: 0.100D-02 0.742D-02 0.497D-02-0.137D-01-0.300D-01-0.132D+00

Coeff: -0.506D-02 0.511D+00 0.656D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=5.13D-09 MaxDP=2.57D-07 DE=-7.09D-11 OVMax= 2.07D-06

Error on total polarization charges = 0.07907

SCF Done: E(UB3LYP) = -1914.20112123 A.U. after 15 cycles

NFock= 15 Conv=0.51D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7877 S= 0.5187

<L.S>= 0.000000000000E+00

KE= 1.906170489854D+03 PE=-1.515316303155D+04 EE= 5.963488294971D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.37

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7877, after 0.7512

Leave Link 502 at Sun Aug 18 14:20:13 2019, MaxMem= 2013265920 cpu: 2811.8

(Enter /home/kira/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

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

GePol: Maximum number of non-zero 1st derivatives = 190

Leave Link 701 at Sun Aug 18 14:20:31 2019, MaxMem= 2013265920 cpu: 142.3

(Enter /home/kira/g09/l702.exe)

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

Leave Link 702 at Sun Aug 18 14:20:31 2019, MaxMem= 2013265920 cpu: 0.1

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

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

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

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Sun Aug 18 14:21:10 2019, MaxMem= 2013265920 cpu: 311.6

(Enter /home/kira/g09/l716.exe)

Dipole = 1.13429674D-13-1.28963507D-12-2.29894355D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000838854 0.000374877 0.000156511

2 6 -0.001218131 -0.000429811 -0.000476996

3 7 0.000000000 -0.000320300 0.000189963

4 6 0.001218131 -0.000429811 -0.000476996

5 6 -0.000838854 0.000374877 0.000156511

6 6 -0.000776938 0.000032289 0.000103888

7 6 -0.000343999 -0.000264560 0.000729331

8 7 -0.000100680 -0.000000000 -0.001157131

9 6 -0.000343999 0.000264560 0.000729331

10 6 0.000146200 -0.000098541 -0.000170175

11 6 0.000146200 0.000098541 -0.000170175

12 6 0.000776938 0.000032289 0.000103888

13 6 0.000343999 -0.000264560 0.000729331

14 6 -0.000146200 0.000098541 -0.000170175

15 6 -0.000146200 -0.000098541 -0.000170175

16 6 0.000343999 0.000264560 0.000729331

17 7 0.000100680 -0.000000000 -0.001157131

18 6 0.000776938 -0.000032289 0.000103888

19 6 -0.001218131 0.000429811 -0.000476996

20 6 0.000838854 -0.000374877 0.000156511

21 6 -0.000838854 -0.000374877 0.000156511

22 6 0.001218131 0.000429811 -0.000476996

23 7 -0.000000000 0.000320300 0.000189963

24 6 -0.000776938 -0.000032289 0.000103888

25 6 0.000287850 0.000199146 -0.000008904

26 6 0.000157099 -0.000136134 0.000185389

27 6 0.000033983 0.000014165 -0.000029879

28 6 0.000029963 0.000015673 -0.000001073

29 6 -0.000020768 0.000043715 0.000035967

30 6 -0.000143617 0.000151633 -0.000220103

31 6 -0.000029963 0.000015673 -0.000001073

32 6 -0.000033983 0.000014165 -0.000029879

33 6 -0.000157099 -0.000136134 0.000185389

34 6 -0.000287850 0.000199146 -0.000008904

35 6 0.000143617 0.000151633 -0.000220103

36 6 0.000020768 0.000043715 0.000035967

37 6 0.000287850 -0.000199146 -0.000008904

38 6 -0.000143617 -0.000151633 -0.000220103

39 6 -0.000020768 -0.000043715 0.000035967

40 6 0.000029963 -0.000015673 -0.000001073

41 6 0.000033983 -0.000014165 -0.000029879

42 6 0.000157099 0.000136134 0.000185389

43 6 -0.000287850 -0.000199146 -0.000008904

44 6 0.000143617 -0.000151633 -0.000220103

45 6 0.000020768 -0.000043715 0.000035967

46 6 -0.000029963 -0.000015673 -0.000001073

47 6 -0.000033983 -0.000014165 -0.000029879

48 6 -0.000157099 0.000136134 0.000185389

49 1 -0.000090356 -0.000028431 0.000061075

50 1 0.000090356 -0.000028431 0.000061075

51 1 -0.000013142 -0.000060107 -0.000032397

52 1 -0.000013142 0.000060107 -0.000032397

53 1 0.000013142 0.000060107 -0.000032397

54 1 0.000013142 -0.000060107 -0.000032397

55 1 -0.000090356 0.000028431 0.000061075

56 1 0.000090356 0.000028431 0.000061075

57 1 -0.000222861 -0.000027941 0.000001606

58 1 -0.000042540 0.000049737 0.000020039

59 1 0.000001852 0.000000745 -0.000001967

60 1 0.000046326 -0.000045251 -0.000016176

61 1 -0.000022488 -0.000214088 -0.000036500

62 1 -0.000001852 0.000000745 -0.000001967

63 1 0.000042540 0.000049737 0.000020039

64 1 0.000222861 -0.000027941 0.000001606

65 1 0.000022488 -0.000214088 -0.000036500

66 1 -0.000046326 -0.000045251 -0.000016176

67 1 -0.000022488 0.000214088 -0.000036500

68 1 0.000046326 0.000045251 -0.000016176

69 1 0.000001852 -0.000000745 -0.000001967

70 1 -0.000042540 -0.000049737 0.000020039

71 1 -0.000222861 0.000027941 0.000001606

72 1 0.000022488 0.000214088 -0.000036500

73 1 -0.000046326 0.000045251 -0.000016176

74 1 -0.000001852 -0.000000745 -0.000001967

75 1 0.000042540 -0.000049737 0.000020039

76 1 0.000222861 0.000027941 0.000001606

77 1 0.000000000 0.000081561 0.000367896

78 1 -0.000000000 -0.000081561 0.000367896

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

Cartesian Forces: Max 0.001218131 RMS 0.000303809

Leave Link 716 at Sun Aug 18 14:21:10 2019, MaxMem= 2013265920 cpu: 0.2

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

Internal Forces: Max 0.000943688 RMS 0.000166213

Search for a local minimum.

Step number 6 out of a maximum of 452

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

RMS Force = .16621D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 2 3 4 5 6

DE= -3.06D-04 DEPred=-2.50D-04 R= 1.22D+00

TightC=F SS= 1.41D+00 RLast= 3.87D-01 DXNew= 7.9759D-01 1.1618D+00

Trust test= 1.22D+00 RLast= 3.87D-01 DXMaxT set to 7.98D-01

ITU= 1 -1 1 1 1 0

Eigenvalues --- 0.00555 0.00861 0.00861 0.00861 0.01613

Eigenvalues --- 0.01654 0.01669 0.01671 0.01686 0.01691

Eigenvalues --- 0.01711 0.01711 0.01711 0.01714 0.01733

Eigenvalues --- 0.01739 0.01758 0.01829 0.01857 0.01869

Eigenvalues --- 0.01887 0.01908 0.01909 0.01909 0.01949

Eigenvalues --- 0.01957 0.02007 0.02008 0.02021 0.02024

Eigenvalues --- 0.02028 0.02041 0.02057 0.02065 0.02078

Eigenvalues --- 0.02080 0.02092 0.02099 0.02099 0.02099

Eigenvalues --- 0.02099 0.02125 0.02132 0.02132 0.02132

Eigenvalues --- 0.02141 0.02141 0.02141 0.02141 0.02161

Eigenvalues --- 0.02161 0.02161 0.02165 0.02165 0.02165

Eigenvalues --- 0.02165 0.02169 0.02171 0.02171 0.02171

Eigenvalues --- 0.02171 0.02175 0.02175 0.02175 0.02176

Eigenvalues --- 0.02176 0.02176 0.02176 0.02202 0.02212

Eigenvalues --- 0.02216 0.02225 0.02230 0.03055 0.04125

Eigenvalues --- 0.15657 0.15983 0.15983 0.15987 0.15988

Eigenvalues --- 0.15991 0.15993 0.15993 0.15993 0.15993

Eigenvalues --- 0.15994 0.15994 0.15994 0.15994 0.15996

Eigenvalues --- 0.15999 0.15999 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16052 0.16249

Eigenvalues --- 0.20250 0.21999 0.21999 0.21999 0.22000

Eigenvalues --- 0.22000 0.22000 0.22001 0.22014 0.22751

Eigenvalues --- 0.22790 0.22795 0.22802 0.23475 0.23475

Eigenvalues --- 0.23475 0.23531 0.23772 0.23996 0.24520

Eigenvalues --- 0.24705 0.24752 0.24785 0.24996 0.24996

Eigenvalues --- 0.24997 0.24998 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25002 0.25084

Eigenvalues --- 0.26240 0.27308 0.33064 0.33146 0.33146

Eigenvalues --- 0.33146 0.34574 0.34603 0.35400 0.35400

Eigenvalues --- 0.35400 0.35400 0.35400 0.35400 0.35400

Eigenvalues --- 0.35404 0.35405 0.35405 0.35405 0.35420

Eigenvalues --- 0.35452 0.35452 0.35452 0.35457 0.35461

Eigenvalues --- 0.35461 0.35461 0.35587 0.36108 0.36108

Eigenvalues --- 0.36108 0.36125 0.36232 0.36232 0.36232

Eigenvalues --- 0.36252 0.36873 0.37022 0.37382 0.37410

Eigenvalues --- 0.39526 0.39578 0.41212 0.41996 0.41996

Eigenvalues --- 0.41996 0.42161 0.42161 0.42161 0.42164

Eigenvalues --- 0.42844 0.43256 0.43501 0.44380 0.44414

Eigenvalues --- 0.44831 0.45322 0.45450 0.45484 0.45544

Eigenvalues --- 0.45632 0.45856 0.45856 0.45856 0.45861

Eigenvalues --- 0.46150 0.46150 0.46150 0.46251 0.46276

Eigenvalues --- 0.46645 0.46645 0.46645 0.46645 0.46834

Eigenvalues --- 0.46834 0.46834 0.47133 0.47485 0.48575

Eigenvalues --- 0.48627 0.49483 0.49746 0.49858 0.50647

Eigenvalues --- 0.52456 0.53081 0.57792

En-DIIS/RFO-DIIS IScMMF= 0 using points: 6 5 4 3 2

RFO step: Lambda=-4.00121629D-05.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 4.52D-04 SmlDif= 1.00D-05

RMS Error= 0.7447071974D-03 NUsed= 5 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.65480 0.50510 -0.55708 0.08915 0.30803

Iteration 1 RMS(Cart)= 0.01918584 RMS(Int)= 0.00024269

Iteration 2 RMS(Cart)= 0.00017089 RMS(Int)= 0.00022204

Iteration 3 RMS(Cart)= 0.00000002 RMS(Int)= 0.00022204

ITry= 1 IFail=0 DXMaxC= 5.37D-02 DCOld= 1.00D+10 DXMaxT= 7.98D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.12D-08 for atom 52.

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

(Linear) (Quad) (Total)

R1 2.69350 0.00046 0.00081 0.00074 0.00145 2.69495

R2 2.59766 -0.00044 -0.00012 -0.00078 -0.00122 2.59645

R3 2.03600 0.00005 0.00010 0.00019 0.00028 2.03629

R4 2.59013 0.00001 0.00006 0.00006 0.00039 2.59052

R5 2.67342 -0.00094 -0.00128 -0.00092 -0.00220 2.67122

R6 2.59013 0.00001 0.00006 0.00006 0.00039 2.59052

R7 1.91057 -0.00015 0.00027 -0.00121 -0.00094 1.90963

R8 2.69350 0.00046 0.00081 0.00074 0.00145 2.69495

R9 2.67342 -0.00094 -0.00128 -0.00092 -0.00220 2.67122

R10 2.03600 0.00005 0.00010 0.00019 0.00028 2.03629

R11 2.66555 -0.00018 -0.00066 0.00107 0.00041 2.66596

R12 2.79880 0.00011 -0.00007 -0.00012 -0.00020 2.79860

R13 2.58236 -0.00021 -0.00063 0.00004 -0.00033 2.58203

R14 2.74942 0.00012 0.00049 0.00010 0.00050 2.74992

R15 2.58236 -0.00021 -0.00063 0.00004 -0.00033 2.58203

R16 2.74942 0.00012 0.00049 0.00010 0.00050 2.74992

R17 2.66555 -0.00018 -0.00066 0.00107 0.00041 2.66596

R18 2.56167 -0.00002 -0.00007 0.00065 0.00025 2.56192

R19 2.03809 0.00003 0.00007 0.00017 0.00024 2.03833

R20 2.03809 0.00003 0.00007 0.00017 0.00024 2.03833

R21 2.66555 -0.00018 -0.00066 0.00107 0.00041 2.66596

R22 2.79880 0.00011 -0.00007 -0.00012 -0.00020 2.79860

R23 2.74942 0.00012 0.00049 0.00010 0.00050 2.74992

R24 2.58236 -0.00021 -0.00063 0.00004 -0.00033 2.58203

R25 2.56167 -0.00002 -0.00007 0.00065 0.00025 2.56192

R26 2.03809 0.00003 0.00007 0.00017 0.00024 2.03833

R27 2.74942 0.00012 0.00049 0.00010 0.00050 2.74992

R28 2.03809 0.00003 0.00007 0.00017 0.00024 2.03833

R29 2.58236 -0.00021 -0.00063 0.00004 -0.00033 2.58203

R30 2.66555 -0.00018 -0.00066 0.00107 0.00041 2.66596

R31 2.67342 -0.00094 -0.00128 -0.00092 -0.00220 2.67122

R32 2.79880 0.00011 -0.00007 -0.00012 -0.00020 2.79860

R33 2.69350 0.00046 0.00081 0.00074 0.00145 2.69495

R34 2.59013 0.00001 0.00006 0.00006 0.00039 2.59052

R35 2.59766 -0.00044 -0.00012 -0.00078 -0.00122 2.59645

R36 2.03600 0.00005 0.00010 0.00019 0.00028 2.03629

R37 2.69350 0.00046 0.00081 0.00074 0.00145 2.69495

R38 2.03600 0.00005 0.00010 0.00019 0.00028 2.03629

R39 2.59013 0.00001 0.00006 0.00006 0.00039 2.59052

R40 2.67342 -0.00094 -0.00128 -0.00092 -0.00220 2.67122

R41 1.91057 -0.00015 0.00027 -0.00121 -0.00094 1.90963

R42 2.79880 0.00011 -0.00007 -0.00012 -0.00020 2.79860

R43 2.65097 -0.00022 -0.00007 -0.00003 -0.00010 2.65087

R44 2.65112 -0.00028 -0.00008 -0.00010 -0.00018 2.65094

R45 2.62830 0.00005 -0.00017 0.00008 -0.00009 2.62821

R46 2.04785 0.00016 0.00021 0.00006 0.00028 2.04812

R47 2.63501 0.00005 0.00007 0.00006 0.00014 2.63515

R48 2.04944 0.00002 0.00002 -0.00001 0.00001 2.04945

R49 2.63549 0.00004 0.00008 0.00004 0.00012 2.63562

R50 2.04977 0.00000 -0.00001 0.00002 0.00001 2.04978

R51 2.62779 0.00004 -0.00018 0.00007 -0.00010 2.62769

R52 2.04945 0.00002 0.00003 -0.00002 0.00001 2.04946

R53 2.04769 0.00013 0.00016 0.00008 0.00024 2.04793

R54 2.63501 0.00005 0.00007 0.00006 0.00014 2.63515

R55 2.63549 0.00004 0.00008 0.00004 0.00012 2.63562

R56 2.04977 0.00000 -0.00001 0.00002 0.00001 2.04978

R57 2.62830 0.00005 -0.00017 0.00008 -0.00009 2.62821

R58 2.04944 0.00002 0.00002 -0.00001 0.00001 2.04945

R59 2.65097 -0.00022 -0.00007 -0.00003 -0.00010 2.65087

R60 2.04785 0.00016 0.00021 0.00006 0.00028 2.04812

R61 2.65112 -0.00028 -0.00008 -0.00010 -0.00018 2.65094

R62 2.62779 0.00004 -0.00018 0.00007 -0.00010 2.62769

R63 2.04769 0.00013 0.00016 0.00008 0.00024 2.04793

R64 2.04945 0.00002 0.00003 -0.00002 0.00001 2.04946

R65 2.65112 -0.00028 -0.00008 -0.00010 -0.00018 2.65094

R66 2.65097 -0.00022 -0.00007 -0.00003 -0.00010 2.65087

R67 2.62779 0.00004 -0.00018 0.00007 -0.00010 2.62769

R68 2.04769 0.00013 0.00016 0.00008 0.00024 2.04793

R69 2.63549 0.00004 0.00008 0.00004 0.00012 2.63562

R70 2.04945 0.00002 0.00003 -0.00002 0.00001 2.04946

R71 2.63501 0.00005 0.00007 0.00006 0.00014 2.63515

R72 2.04977 0.00000 -0.00001 0.00002 0.00001 2.04978

R73 2.62830 0.00005 -0.00017 0.00008 -0.00009 2.62821

R74 2.04944 0.00002 0.00002 -0.00001 0.00001 2.04945

R75 2.04785 0.00016 0.00021 0.00006 0.00028 2.04812

R76 2.65112 -0.00028 -0.00008 -0.00010 -0.00018 2.65094

R77 2.65097 -0.00022 -0.00007 -0.00003 -0.00010 2.65087

R78 2.62779 0.00004 -0.00018 0.00007 -0.00010 2.62769

R79 2.04769 0.00013 0.00016 0.00008 0.00024 2.04793

R80 2.63549 0.00004 0.00008 0.00004 0.00012 2.63562

R81 2.04945 0.00002 0.00003 -0.00002 0.00001 2.04946

R82 2.63501 0.00005 0.00007 0.00006 0.00014 2.63515

R83 2.04977 0.00000 -0.00001 0.00002 0.00001 2.04978

R84 2.62830 0.00005 -0.00017 0.00008 -0.00009 2.62821

R85 2.04944 0.00002 0.00002 -0.00001 0.00001 2.04945

R86 2.04785 0.00016 0.00021 0.00006 0.00028 2.04812

A1 1.88269 0.00004 -0.00026 0.00071 0.00056 1.88325

A2 2.18408 -0.00010 0.00027 -0.00115 -0.00093 2.18315

A3 2.21606 0.00007 -0.00000 0.00046 0.00041 2.21647

A4 1.86707 -0.00005 0.00048 -0.00181 -0.00127 1.86580

A5 2.21114 0.00029 0.00125 0.00231 0.00266 2.21381

A6 2.20490 -0.00023 -0.00176 -0.00047 -0.00141 2.20349

A7 1.92479 0.00002 -0.00070 0.00216 0.00128 1.92607

A8 2.17917 -0.00001 0.00032 -0.00108 -0.00063 2.17854

A9 2.17917 -0.00001 0.00032 -0.00108 -0.00063 2.17854

A10 1.86707 -0.00005 0.00048 -0.00181 -0.00127 1.86580

A11 2.20490 -0.00023 -0.00176 -0.00047 -0.00141 2.20349

A12 2.21114 0.00029 0.00125 0.00231 0.00266 2.21381

A13 1.88269 0.00004 -0.00026 0.00071 0.00056 1.88325

A14 2.21606 0.00007 -0.00000 0.00046 0.00041 2.21647

A15 2.18408 -0.00010 0.00027 -0.00115 -0.00093 2.18315

A16 2.18365 -0.00003 -0.00271 0.00073 -0.00081 2.18284

A17 2.03607 0.00006 0.00116 -0.00015 0.00043 2.03650

A18 2.06346 -0.00003 0.00156 -0.00059 0.00038 2.06384

A19 2.18462 0.00013 -0.00178 0.00149 0.00053 2.18515

A20 2.16407 -0.00031 0.00082 -0.00023 -0.00031 2.16376

A21 1.93435 0.00017 0.00091 -0.00127 -0.00026 1.93410

A22 1.84210 -0.00014 -0.00116 0.00176 0.00039 1.84249

A23 1.93435 0.00017 0.00091 -0.00127 -0.00026 1.93410

A24 2.18462 0.00013 -0.00178 0.00149 0.00053 2.18515

A25 2.16407 -0.00031 0.00082 -0.00023 -0.00031 2.16376

A26 1.85667 -0.00011 -0.00057 0.00040 -0.00009 1.85659

A27 2.20023 0.00000 0.00052 -0.00082 -0.00035 2.19989

A28 2.22581 0.00011 0.00009 0.00045 0.00050 2.22631

A29 1.85667 -0.00011 -0.00057 0.00040 -0.00009 1.85659

A30 2.20023 0.00000 0.00052 -0.00082 -0.00035 2.19989

A31 2.22581 0.00011 0.00009 0.00045 0.00050 2.22631

A32 2.18365 -0.00003 -0.00271 0.00073 -0.00081 2.18284

A33 2.03607 0.00006 0.00116 -0.00015 0.00043 2.03650

A34 2.06346 -0.00003 0.00156 -0.00059 0.00038 2.06384

A35 2.16407 -0.00031 0.00082 -0.00023 -0.00031 2.16376

A36 2.18462 0.00013 -0.00178 0.00149 0.00053 2.18515

A37 1.93435 0.00017 0.00091 -0.00127 -0.00026 1.93410

A38 1.85667 -0.00011 -0.00057 0.00040 -0.00009 1.85659

A39 2.20023 0.00000 0.00052 -0.00082 -0.00035 2.19989

A40 2.22581 0.00011 0.00009 0.00045 0.00050 2.22631

A41 1.85667 -0.00011 -0.00057 0.00040 -0.00009 1.85659

A42 2.22581 0.00011 0.00009 0.00045 0.00050 2.22631

A43 2.20023 0.00000 0.00052 -0.00082 -0.00035 2.19989

A44 1.93435 0.00017 0.00091 -0.00127 -0.00026 1.93410

A45 2.16407 -0.00031 0.00082 -0.00023 -0.00031 2.16376

A46 2.18462 0.00013 -0.00178 0.00149 0.00053 2.18515

A47 1.84210 -0.00014 -0.00116 0.00176 0.00039 1.84249

A48 2.18365 -0.00003 -0.00271 0.00073 -0.00081 2.18284

A49 2.06346 -0.00003 0.00156 -0.00059 0.00038 2.06384

A50 2.03607 0.00006 0.00116 -0.00015 0.00043 2.03650

A51 2.21114 0.00029 0.00125 0.00231 0.00266 2.21381

A52 2.20490 -0.00023 -0.00176 -0.00047 -0.00141 2.20349

A53 1.86707 -0.00005 0.00048 -0.00181 -0.00127 1.86580

A54 1.88269 0.00004 -0.00026 0.00071 0.00056 1.88325

A55 2.18408 -0.00010 0.00027 -0.00115 -0.00093 2.18315

A56 2.21606 0.00007 -0.00000 0.00046 0.00041 2.21647

A57 1.88269 0.00004 -0.00026 0.00071 0.00056 1.88325

A58 2.21606 0.00007 -0.00000 0.00046 0.00041 2.21647

A59 2.18408 -0.00010 0.00027 -0.00115 -0.00093 2.18315

A60 1.86707 -0.00005 0.00048 -0.00181 -0.00127 1.86580

A61 2.21114 0.00029 0.00125 0.00231 0.00266 2.21381

A62 2.20490 -0.00023 -0.00176 -0.00047 -0.00141 2.20349

A63 1.92479 0.00002 -0.00070 0.00216 0.00128 1.92607

A64 2.17917 -0.00001 0.00032 -0.00108 -0.00063 2.17854

A65 2.17917 -0.00001 0.00032 -0.00108 -0.00063 2.17854

A66 2.18365 -0.00003 -0.00271 0.00073 -0.00081 2.18284

A67 2.06346 -0.00003 0.00156 -0.00059 0.00038 2.06384

A68 2.03607 0.00006 0.00116 -0.00015 0.00043 2.03650

A69 2.10467 -0.00005 -0.00004 0.00015 0.00011 2.10478

A70 2.09872 -0.00003 0.00014 0.00043 0.00056 2.09929

A71 2.07980 0.00008 -0.00009 -0.00058 -0.00067 2.07912

A72 2.09965 0.00002 0.00015 0.00038 0.00053 2.10018

A73 2.08758 -0.00012 -0.00020 -0.00002 -0.00021 2.08738

A74 2.09558 0.00010 0.00005 -0.00036 -0.00029 2.09529

A75 2.09717 -0.00005 -0.00012 0.00005 -0.00006 2.09711

A76 2.08874 0.00002 -0.00002 -0.00005 -0.00007 2.08867

A77 2.09727 0.00004 0.00014 0.00000 0.00014 2.09741

A78 2.09260 -0.00004 0.00006 -0.00032 -0.00026 2.09234

A79 2.09532 0.00002 -0.00003 0.00016 0.00012 2.09544

A80 2.09526 0.00002 -0.00002 0.00016 0.00014 2.09540

A81 2.09718 -0.00004 -0.00010 0.00004 -0.00006 2.09713

A82 2.09718 0.00003 0.00013 0.00001 0.00015 2.09732

A83 2.08882 0.00000 -0.00003 -0.00006 -0.00009 2.08873

A84 2.09972 0.00003 0.00014 0.00041 0.00055 2.10027

A85 2.08687 -0.00013 -0.00020 -0.00009 -0.00028 2.08659

A86 2.09625 0.00010 0.00007 -0.00033 -0.00025 2.09600

A87 2.09260 -0.00004 0.00006 -0.00032 -0.00026 2.09234

A88 2.09532 0.00002 -0.00003 0.00016 0.00012 2.09544

A89 2.09526 0.00002 -0.00002 0.00016 0.00014 2.09540

A90 2.09717 -0.00005 -0.00012 0.00005 -0.00006 2.09711

A91 2.09727 0.00004 0.00014 0.00000 0.00014 2.09741

A92 2.08874 0.00002 -0.00002 -0.00005 -0.00007 2.08867

A93 2.09965 0.00002 0.00015 0.00038 0.00053 2.10018

A94 2.09558 0.00010 0.00005 -0.00036 -0.00029 2.09529

A95 2.08758 -0.00012 -0.00020 -0.00002 -0.00021 2.08738

A96 2.10467 -0.00005 -0.00004 0.00015 0.00011 2.10478

A97 2.09872 -0.00003 0.00014 0.00043 0.00056 2.09929

A98 2.07980 0.00008 -0.00009 -0.00058 -0.00067 2.07912

A99 2.09972 0.00003 0.00014 0.00041 0.00055 2.10027

A100 2.08687 -0.00013 -0.00020 -0.00009 -0.00028 2.08659

A101 2.09625 0.00010 0.00007 -0.00033 -0.00025 2.09600

A102 2.09718 -0.00004 -0.00010 0.00004 -0.00006 2.09713

A103 2.09718 0.00003 0.00013 0.00001 0.00015 2.09732

A104 2.08882 0.00000 -0.00003 -0.00006 -0.00009 2.08873

A105 2.09872 -0.00003 0.00014 0.00043 0.00056 2.09929

A106 2.10467 -0.00005 -0.00004 0.00015 0.00011 2.10478

A107 2.07980 0.00008 -0.00009 -0.00058 -0.00067 2.07912

A108 2.09972 0.00003 0.00014 0.00041 0.00055 2.10027

A109 2.08687 -0.00013 -0.00020 -0.00009 -0.00028 2.08659

A110 2.09625 0.00010 0.00007 -0.00033 -0.00025 2.09600

A111 2.09718 -0.00004 -0.00010 0.00004 -0.00006 2.09713

A112 2.08882 0.00000 -0.00003 -0.00006 -0.00009 2.08873

A113 2.09718 0.00003 0.00013 0.00001 0.00015 2.09732

A114 2.09260 -0.00004 0.00006 -0.00032 -0.00026 2.09234

A115 2.09526 0.00002 -0.00002 0.00016 0.00014 2.09540

A116 2.09532 0.00002 -0.00003 0.00016 0.00012 2.09544

A117 2.09717 -0.00005 -0.00012 0.00005 -0.00006 2.09711

A118 2.09727 0.00004 0.00014 0.00000 0.00014 2.09741

A119 2.08874 0.00002 -0.00002 -0.00005 -0.00007 2.08867

A120 2.09965 0.00002 0.00015 0.00038 0.00053 2.10018

A121 2.08758 -0.00012 -0.00020 -0.00002 -0.00021 2.08738

A122 2.09558 0.00010 0.00005 -0.00036 -0.00029 2.09529

A123 2.09872 -0.00003 0.00014 0.00043 0.00056 2.09929

A124 2.10467 -0.00005 -0.00004 0.00015 0.00011 2.10478

A125 2.07980 0.00008 -0.00009 -0.00058 -0.00067 2.07912

A126 2.09972 0.00003 0.00014 0.00041 0.00055 2.10027

A127 2.08687 -0.00013 -0.00020 -0.00009 -0.00028 2.08659

A128 2.09625 0.00010 0.00007 -0.00033 -0.00025 2.09600

A129 2.09718 -0.00004 -0.00010 0.00004 -0.00006 2.09713

A130 2.08882 0.00000 -0.00003 -0.00006 -0.00009 2.08873

A131 2.09718 0.00003 0.00013 0.00001 0.00015 2.09732

A132 2.09260 -0.00004 0.00006 -0.00032 -0.00026 2.09234

A133 2.09526 0.00002 -0.00002 0.00016 0.00014 2.09540

A134 2.09532 0.00002 -0.00003 0.00016 0.00012 2.09544

A135 2.09717 -0.00005 -0.00012 0.00005 -0.00006 2.09711

A136 2.09727 0.00004 0.00014 0.00000 0.00014 2.09741

A137 2.08874 0.00002 -0.00002 -0.00005 -0.00007 2.08867

A138 2.09965 0.00002 0.00015 0.00038 0.00053 2.10018

A139 2.08758 -0.00012 -0.00020 -0.00002 -0.00021 2.08738

A140 2.09558 0.00010 0.00005 -0.00036 -0.00029 2.09529

D1 0.01682 0.00018 0.00156 0.00109 0.00268 0.01951

D2 -3.11255 0.00018 0.00483 -0.00046 0.00446 -3.10809

D3 -3.09774 0.00009 0.00033 0.00061 0.00094 -3.09680

D4 0.05607 0.00010 0.00361 -0.00093 0.00271 0.05878

D5 0.00000 0.00000 -0.00000 -0.00000 0.00000 0.00000

D6 -3.11393 -0.00008 -0.00128 -0.00045 -0.00176 -3.11569

D7 3.11393 0.00008 0.00128 0.00045 0.00176 3.11569

D8 -0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 -0.02802 -0.00029 -0.00260 -0.00185 -0.00450 -0.03251

D10 3.10246 -0.00013 -0.00015 -0.00268 -0.00280 3.09965

D11 3.10141 -0.00030 -0.00584 -0.00028 -0.00622 3.09519

D12 -0.05130 -0.00014 -0.00338 -0.00112 -0.00453 -0.05583

D13 -2.98273 -0.00004 -0.00120 0.00317 0.00199 -2.98075

D14 0.15377 0.00000 0.00060 0.00079 0.00141 0.15518

D15 0.17336 -0.00003 0.00267 0.00134 0.00408 0.17745

D16 -2.97332 0.00001 0.00446 -0.00104 0.00351 -2.96981

D17 0.02802 0.00029 0.00260 0.00185 0.00450 0.03251

D18 -3.10141 0.00030 0.00584 0.00028 0.00622 -3.09519

D19 -3.10246 0.00013 0.00015 0.00268 0.00280 -3.09965

D20 0.05130 0.00014 0.00338 0.00112 0.00453 0.05583

D21 -0.01682 -0.00018 -0.00156 -0.00109 -0.00268 -0.01951

D22 3.09774 -0.00009 -0.00033 -0.00061 -0.00094 3.09680

D23 3.11255 -0.00018 -0.00483 0.00046 -0.00446 3.10809

D24 -0.05607 -0.00010 -0.00361 0.00093 -0.00271 -0.05878

D25 -0.17336 0.00003 -0.00267 -0.00134 -0.00408 -0.17745

D26 2.97332 -0.00001 -0.00446 0.00104 -0.00351 2.96981

D27 2.98273 0.00004 0.00120 -0.00317 -0.00199 2.98075

D28 -0.15377 -0.00000 -0.00060 -0.00079 -0.00141 -0.15518

D29 -0.16858 0.00004 -0.00281 0.00078 -0.00211 -0.17069

D30 2.99260 -0.00000 -0.00203 0.00217 0.00013 2.99273

D31 2.96785 0.00009 -0.00099 -0.00163 -0.00270 2.96515

D32 -0.15416 0.00004 -0.00021 -0.00024 -0.00046 -0.15461

D33 -0.99160 0.00030 0.00819 0.00214 0.01033 -0.98128

D34 2.15024 0.00030 0.00765 0.00242 0.01007 2.16031

D35 2.15471 0.00026 0.00652 0.00434 0.01087 2.16558

D36 -0.98663 0.00026 0.00598 0.00463 0.01061 -0.97601

D37 -3.09170 0.00037 0.00783 0.00100 0.00898 -3.08272

D38 0.03252 0.00041 0.00719 -0.00023 0.00699 0.03951

D39 3.10396 -0.00022 -0.00526 -0.00103 -0.00635 3.09761

D40 -0.06865 -0.00008 -0.00383 -0.00027 -0.00413 -0.07278

D41 -0.02050 -0.00026 -0.00454 0.00016 -0.00440 -0.02490

D42 3.09008 -0.00012 -0.00310 0.00091 -0.00218 3.08790

D43 -0.03252 -0.00041 -0.00719 0.00023 -0.00699 -0.03951

D44 3.09170 -0.00037 -0.00783 -0.00100 -0.00898 3.08272

D45 0.02050 0.00026 0.00454 -0.00016 0.00440 0.02490

D46 -3.09008 0.00012 0.00310 -0.00091 0.00218 -3.08790

D47 -3.10396 0.00022 0.00526 0.00103 0.00635 -3.09761

D48 0.06865 0.00008 0.00383 0.00027 0.00413 0.07278

D49 0.16858 -0.00004 0.00281 -0.00078 0.00211 0.17069

D50 -2.96785 -0.00009 0.00099 0.00163 0.00270 -2.96515

D51 -2.99260 0.00000 0.00203 -0.00217 -0.00013 -2.99273

D52 0.15416 -0.00004 0.00021 0.00024 0.00046 0.15461

D53 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D54 -3.10998 -0.00014 -0.00148 -0.00074 -0.00224 -3.11222

D55 3.10998 0.00014 0.00148 0.00074 0.00224 3.11222

D56 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D57 -2.99260 0.00000 0.00203 -0.00217 -0.00013 -2.99273

D58 0.16858 -0.00004 0.00281 -0.00078 0.00211 0.17069

D59 0.15416 -0.00004 0.00021 0.00024 0.00046 0.15461

D60 -2.96785 -0.00009 0.00099 0.00163 0.00270 -2.96515

D61 0.99160 -0.00030 -0.00819 -0.00214 -0.01033 0.98128

D62 -2.15024 -0.00030 -0.00765 -0.00242 -0.01007 -2.16031

D63 -2.15471 -0.00026 -0.00652 -0.00434 -0.01087 -2.16558

D64 0.98663 -0.00026 -0.00598 -0.00463 -0.01061 0.97601

D65 -3.10396 0.00022 0.00526 0.00103 0.00635 -3.09761

D66 0.06865 0.00008 0.00383 0.00027 0.00413 0.07278

D67 0.02050 0.00026 0.00454 -0.00016 0.00440 0.02490

D68 -3.09008 0.00012 0.00310 -0.00091 0.00218 -3.08790

D69 3.09170 -0.00037 -0.00783 -0.00100 -0.00898 3.08272

D70 -0.03252 -0.00041 -0.00719 0.00023 -0.00699 -0.03951

D71 -0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D72 -3.10998 -0.00014 -0.00148 -0.00074 -0.00224 -3.11222

D73 3.10998 0.00014 0.00148 0.00074 0.00224 3.11222

D74 0.00000 -0.00000 -0.00000 -0.00000 0.00000 0.00000

D75 -0.02050 -0.00026 -0.00454 0.00016 -0.00440 -0.02490

D76 3.10396 -0.00022 -0.00526 -0.00103 -0.00635 3.09761

D77 3.09008 -0.00012 -0.00310 0.00091 -0.00218 3.08790

D78 -0.06865 -0.00008 -0.00383 -0.00027 -0.00413 -0.07278

D79 0.03252 0.00041 0.00719 -0.00023 0.00699 0.03951

D80 -3.09170 0.00037 0.00783 0.00100 0.00898 -3.08272

D81 2.99260 -0.00000 -0.00203 0.00217 0.00013 2.99273

D82 -0.15416 0.00004 -0.00021 -0.00024 -0.00046 -0.15461

D83 -0.16858 0.00004 -0.00281 0.00078 -0.00211 -0.17069

D84 2.96785 0.00009 -0.00099 -0.00163 -0.00270 2.96515

D85 2.98273 0.00004 0.00120 -0.00317 -0.00199 2.98075

D86 -0.17336 0.00003 -0.00267 -0.00134 -0.00408 -0.17745

D87 -0.15377 -0.00000 -0.00060 -0.00079 -0.00141 -0.15518

D88 2.97332 -0.00001 -0.00446 0.00104 -0.00351 2.96981

D89 -0.98663 0.00026 0.00598 0.00463 0.01061 -0.97601

D90 2.15471 0.00026 0.00652 0.00434 0.01087 2.16558

D91 2.15024 0.00030 0.00765 0.00242 0.01007 2.16031

D92 -0.99160 0.00030 0.00819 0.00214 0.01033 -0.98128

D93 3.11255 -0.00018 -0.00483 0.00046 -0.00446 3.10809

D94 -0.05607 -0.00010 -0.00361 0.00093 -0.00271 -0.05878

D95 -0.01682 -0.00018 -0.00156 -0.00109 -0.00268 -0.01951

D96 3.09774 -0.00009 -0.00033 -0.00061 -0.00094 3.09680

D97 -3.10141 0.00030 0.00584 0.00028 0.00622 -3.09519

D98 0.05130 0.00014 0.00338 0.00112 0.00453 0.05583

D99 0.02802 0.00029 0.00260 0.00185 0.00450 0.03251

D100 -3.10246 0.00013 0.00015 0.00268 0.00280 -3.09965

D101 0.00000 -0.00000 -0.00000 -0.00000 0.00000 0.00000

D102 3.11393 0.00008 0.00128 0.00045 0.00176 3.11569

D103 -3.11393 -0.00008 -0.00128 -0.00045 -0.00176 -3.11569

D104 -0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D105 0.01682 0.00018 0.00156 0.00109 0.00268 0.01951

D106 -3.11255 0.00018 0.00483 -0.00046 0.00446 -3.10809

D107 -3.09774 0.00009 0.00033 0.00061 0.00094 -3.09680

D108 0.05607 0.00010 0.00361 -0.00093 0.00271 0.05878

D109 -0.02802 -0.00029 -0.00260 -0.00185 -0.00450 -0.03251

D110 3.10246 -0.00013 -0.00015 -0.00268 -0.00280 3.09965

D111 3.10141 -0.00030 -0.00584 -0.00028 -0.00622 3.09519

D112 -0.05130 -0.00014 -0.00338 -0.00112 -0.00453 -0.05583

D113 -2.98273 -0.00004 -0.00120 0.00317 0.00199 -2.98075

D114 0.15377 0.00000 0.00060 0.00079 0.00141 0.15518

D115 0.17336 -0.00003 0.00267 0.00134 0.00408 0.17745

D116 -2.97332 0.00001 0.00446 -0.00104 0.00351 -2.96981

D117 0.98663 -0.00026 -0.00598 -0.00463 -0.01061 0.97601

D118 -2.15471 -0.00026 -0.00652 -0.00434 -0.01087 -2.16558

D119 -2.15024 -0.00030 -0.00765 -0.00242 -0.01007 -2.16031

D120 0.99160 -0.00030 -0.00819 -0.00214 -0.01033 0.98128

D121 -3.13102 -0.00002 -0.00100 0.00004 -0.00096 -3.13198

D122 -0.01879 0.00006 0.00035 -0.00009 0.00026 -0.01853

D123 0.01032 -0.00002 -0.00047 -0.00024 -0.00071 0.00961

D124 3.12255 0.00006 0.00088 -0.00037 0.00051 3.12306

D125 -3.13294 -0.00001 -0.00056 0.00042 -0.00014 -3.13308

D126 -0.01937 0.00007 0.00101 -0.00026 0.00075 -0.01862

D127 0.00890 -0.00001 -0.00109 0.00070 -0.00039 0.00852

D128 3.12247 0.00008 0.00048 0.00003 0.00050 3.12298

D129 -0.01957 0.00004 0.00147 -0.00029 0.00118 -0.01838

D130 3.12136 0.00006 0.00129 0.00044 0.00173 3.12309

D131 -3.13165 -0.00004 0.00012 -0.00017 -0.00004 -3.13170

D132 0.00927 -0.00003 -0.00006 0.00056 0.00050 0.00977

D133 0.00954 -0.00002 -0.00092 0.00036 -0.00056 0.00898

D134 -3.13193 -0.00002 -0.00082 0.00022 -0.00060 -3.13252

D135 -3.13138 -0.00004 -0.00074 -0.00037 -0.00111 -3.13249

D136 0.01034 -0.00004 -0.00064 -0.00051 -0.00115 0.00919

D137 0.00970 -0.00002 -0.00064 0.00010 -0.00055 0.00916

D138 -3.13112 -0.00004 -0.00054 -0.00058 -0.00112 -3.13224

D139 -3.13202 -0.00002 -0.00074 0.00023 -0.00051 -3.13253

D140 0.01035 -0.00004 -0.00064 -0.00045 -0.00108 0.00926

D141 -0.01893 0.00003 0.00165 -0.00063 0.00102 -0.01791

D142 -3.13235 -0.00005 0.00008 0.00004 0.00012 -3.13223

D143 3.12190 0.00005 0.00154 0.00004 0.00158 3.12348

D144 0.00848 -0.00003 -0.00003 0.00071 0.00069 0.00917

D145 -0.00954 0.00002 0.00092 -0.00036 0.00056 -0.00898

D146 3.13138 0.00004 0.00074 0.00037 0.00111 3.13249

D147 3.13193 0.00002 0.00082 -0.00022 0.00060 3.13252

D148 -0.01034 0.00004 0.00064 0.00051 0.00115 -0.00919

D149 -0.00970 0.00002 0.00064 -0.00010 0.00055 -0.00916

D150 3.13112 0.00004 0.00054 0.00058 0.00112 3.13224

D151 3.13202 0.00002 0.00074 -0.00023 0.00051 3.13253

D152 -0.01035 0.00004 0.00064 0.00045 0.00108 -0.00926

D153 0.01957 -0.00004 -0.00147 0.00029 -0.00118 0.01838

D154 3.13165 0.00004 -0.00012 0.00017 0.00004 3.13170

D155 -3.12136 -0.00006 -0.00129 -0.00044 -0.00173 -3.12309

D156 -0.00927 0.00003 0.00006 -0.00056 -0.00050 -0.00977

D157 3.13102 0.00002 0.00100 -0.00004 0.00096 3.13198

D158 -0.01032 0.00002 0.00047 0.00024 0.00071 -0.00961

D159 0.01879 -0.00006 -0.00035 0.00009 -0.00026 0.01853

D160 -3.12255 -0.00006 -0.00088 0.00037 -0.00051 -3.12306

D161 3.13294 0.00001 0.00056 -0.00042 0.00014 3.13308

D162 0.01937 -0.00007 -0.00101 0.00026 -0.00075 0.01862

D163 -0.00890 0.00001 0.00109 -0.00070 0.00039 -0.00852

D164 -3.12247 -0.00008 -0.00048 -0.00003 -0.00050 -3.12298

D165 0.01893 -0.00003 -0.00165 0.00063 -0.00102 0.01791

D166 -3.12190 -0.00005 -0.00154 -0.00004 -0.00158 -3.12348

D167 3.13235 0.00005 -0.00008 -0.00004 -0.00012 3.13223

D168 -0.00848 0.00003 0.00003 -0.00071 -0.00069 -0.00917

D169 3.13294 0.00001 0.00056 -0.00042 0.00014 3.13308

D170 0.01937 -0.00007 -0.00101 0.00026 -0.00075 0.01862

D171 -0.00890 0.00001 0.00109 -0.00070 0.00039 -0.00852

D172 -3.12247 -0.00008 -0.00048 -0.00003 -0.00050 -3.12298

D173 3.13102 0.00002 0.00100 -0.00004 0.00096 3.13198

D174 0.01879 -0.00006 -0.00035 0.00009 -0.00026 0.01853

D175 -0.01032 0.00002 0.00047 0.00024 0.00071 -0.00961

D176 -3.12255 -0.00006 -0.00088 0.00037 -0.00051 -3.12306

D177 0.01893 -0.00003 -0.00165 0.00063 -0.00102 0.01791

D178 -3.12190 -0.00005 -0.00154 -0.00004 -0.00158 -3.12348

D179 3.13235 0.00005 -0.00008 -0.00004 -0.00012 3.13223

D180 -0.00848 0.00003 0.00003 -0.00071 -0.00069 -0.00917

D181 -0.00970 0.00002 0.00064 -0.00010 0.00055 -0.00916

D182 3.13202 0.00002 0.00074 -0.00023 0.00051 3.13253

D183 3.13112 0.00004 0.00054 0.00058 0.00112 3.13224

D184 -0.01035 0.00004 0.00064 0.00045 0.00108 -0.00926

D185 -0.00954 0.00002 0.00092 -0.00036 0.00056 -0.00898

D186 3.13138 0.00004 0.00074 0.00037 0.00111 3.13249

D187 3.13193 0.00002 0.00082 -0.00022 0.00060 3.13252

D188 -0.01034 0.00004 0.00064 0.00051 0.00115 -0.00919

D189 0.01957 -0.00004 -0.00147 0.00029 -0.00118 0.01838

D190 3.13165 0.00004 -0.00012 0.00017 0.00004 3.13170

D191 -3.12136 -0.00006 -0.00129 -0.00044 -0.00173 -3.12309

D192 -0.00927 0.00003 0.00006 -0.00056 -0.00050 -0.00977

D193 -3.13294 -0.00001 -0.00056 0.00042 -0.00014 -3.13308

D194 -0.01937 0.00007 0.00101 -0.00026 0.00075 -0.01862

D195 0.00890 -0.00001 -0.00109 0.00070 -0.00039 0.00852

D196 3.12247 0.00008 0.00048 0.00003 0.00050 3.12298

D197 -3.13102 -0.00002 -0.00100 0.00004 -0.00096 -3.13198

D198 -0.01879 0.00006 0.00035 -0.00009 0.00026 -0.01853

D199 0.01032 -0.00002 -0.00047 -0.00024 -0.00071 0.00961

D200 3.12255 0.00006 0.00088 -0.00037 0.00051 3.12306

D201 -0.01893 0.00003 0.00165 -0.00063 0.00102 -0.01791

D202 3.12190 0.00005 0.00154 0.00004 0.00158 3.12348

D203 -3.13235 -0.00005 0.00008 0.00004 0.00012 -3.13223

D204 0.00848 -0.00003 -0.00003 0.00071 0.00069 0.00917

D205 0.00970 -0.00002 -0.00064 0.00010 -0.00055 0.00916

D206 -3.13202 -0.00002 -0.00074 0.00023 -0.00051 -3.13253

D207 -3.13112 -0.00004 -0.00054 -0.00058 -0.00112 -3.13224

D208 0.01035 -0.00004 -0.00064 -0.00045 -0.00108 0.00926

D209 0.00954 -0.00002 -0.00092 0.00036 -0.00056 0.00898

D210 -3.13138 -0.00004 -0.00074 -0.00037 -0.00111 -3.13249

D211 -3.13193 -0.00002 -0.00082 0.00022 -0.00060 -3.13252

D212 0.01034 -0.00004 -0.00064 -0.00051 -0.00115 0.00919

D213 -0.01957 0.00004 0.00147 -0.00029 0.00118 -0.01838

D214 -3.13165 -0.00004 0.00012 -0.00017 -0.00004 -3.13170

D215 3.12136 0.00006 0.00129 0.00044 0.00173 3.12309

D216 0.00927 -0.00003 -0.00006 0.00056 0.00050 0.00977

Item Value Threshold Converged?

Maximum Force 0.000944 0.000450 NO

RMS Force 0.000166 0.000300 YES

Maximum Displacement 0.053726 0.001800 NO

RMS Displacement 0.019210 0.001200 NO

Predicted change in Energy=-8.177614D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Aug 18 14:21:11 2019, MaxMem= 2013265920 cpu: 1.5

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

Stoichiometry C44H30N4(1+,2)

Framework group C2V[SGV(H2N2),SGV'(N2),X(C44H28)]

Deg. of freedom 59

Full point group C2V NOp 4

RotChk: IX=0 Diff= 7.99D-17

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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1 6 0 -0.686990 4.182049 0.474298

2 6 0 -1.125366 2.867117 0.138804

3 7 0 0.000000 2.102702 -0.029826

4 6 0 1.125366 2.867117 0.138804

5 6 0 0.686990 4.182049 0.474298

6 6 0 2.461783 2.431741 -0.011383

7 6 0 2.864416 1.088099 -0.162259

8 7 0 2.054500 -0.000000 0.002018

9 6 0 2.864416 -1.088099 -0.162259

10 6 0 4.221032 -0.677855 -0.492245

11 6 0 4.221032 0.677855 -0.492245

12 6 0 -2.461783 2.431741 -0.011383

13 6 0 -2.864416 1.088099 -0.162259

14 6 0 -4.221032 0.677855 -0.492245

15 6 0 -4.221032 -0.677855 -0.492245

16 6 0 -2.864416 -1.088099 -0.162259

17 7 0 -2.054500 0.000000 0.002018

18 6 0 -2.461783 -2.431741 -0.011383

19 6 0 -1.125366 -2.867117 0.138804

20 6 0 -0.686990 -4.182049 0.474298

21 6 0 0.686990 -4.182049 0.474298

22 6 0 1.125366 -2.867117 0.138804

23 7 0 -0.000000 -2.102702 -0.029826

24 6 0 2.461783 -2.431741 -0.011383

25 6 0 3.507905 3.479947 -0.000386

26 6 0 3.458321 4.547682 -0.908829

27 6 0 4.449848 5.522929 -0.901233

28 6 0 5.489719 5.457463 0.025538

29 6 0 5.540621 4.405308 0.939643

30 6 0 4.563281 3.416364 0.921585

31 6 0 -5.489719 5.457463 0.025538

32 6 0 -4.449848 5.522929 -0.901233

33 6 0 -3.458321 4.547682 -0.908829

34 6 0 -3.507905 3.479947 -0.000386

35 6 0 -4.563281 3.416364 0.921585

36 6 0 -5.540621 4.405308 0.939643

37 6 0 3.507905 -3.479947 -0.000386

38 6 0 4.563281 -3.416364 0.921585

39 6 0 5.540621 -4.405308 0.939643

40 6 0 5.489719 -5.457463 0.025538

41 6 0 4.449848 -5.522929 -0.901233

42 6 0 3.458321 -4.547682 -0.908829

43 6 0 -3.507905 -3.479947 -0.000386

44 6 0 -4.563281 -3.416364 0.921585

45 6 0 -5.540621 -4.405308 0.939643

46 6 0 -5.489719 -5.457463 0.025538

47 6 0 -4.449848 -5.522929 -0.901233

48 6 0 -3.458321 -4.547682 -0.908829

49 1 0 -1.335400 5.010180 0.708595

50 1 0 1.335400 5.010180 0.708595

51 1 0 5.045588 -1.335355 -0.718653

52 1 0 5.045588 1.335355 -0.718653

53 1 0 -5.045588 1.335355 -0.718653

54 1 0 -5.045588 -1.335355 -0.718653

55 1 0 -1.335400 -5.010180 0.708595

56 1 0 1.335400 -5.010180 0.708595

57 1 0 2.655899 4.595157 -1.635831

58 1 0 4.410274 6.334382 -1.619677

59 1 0 6.257608 6.223497 0.035572

60 1 0 6.342476 4.354523 1.668096

61 1 0 4.599001 2.603979 1.637964

62 1 0 -6.257608 6.223497 0.035572

63 1 0 -4.410274 6.334382 -1.619677

64 1 0 -2.655899 4.595157 -1.635831

65 1 0 -4.599001 2.603979 1.637964

66 1 0 -6.342476 4.354523 1.668096

67 1 0 4.599001 -2.603979 1.637964

68 1 0 6.342476 -4.354523 1.668096

69 1 0 6.257608 -6.223497 0.035572

70 1 0 4.410274 -6.334382 -1.619677

71 1 0 2.655899 -4.595157 -1.635831

72 1 0 -4.599001 -2.603979 1.637964

73 1 0 -6.342476 -4.354523 1.668096

74 1 0 -6.257608 -6.223497 0.035572

75 1 0 -4.410274 -6.334382 -1.619677

76 1 0 -2.655899 -4.595157 -1.635831

77 1 0 0.000000 1.114241 -0.239870

78 1 0 -0.000000 -1.114241 -0.239870

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Rotational constants (GHZ): 0.0592341 0.0585439 0.0302691

Leave Link 202 at Sun Aug 18 14:21:11 2019, MaxMem= 2013265920 cpu: 0.1

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

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

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

There are 261 symmetry adapted cartesian basis functions of A1 symmetry.

There are 240 symmetry adapted cartesian basis functions of A2 symmetry.

There are 249 symmetry adapted cartesian basis functions of B1 symmetry.

There are 252 symmetry adapted cartesian basis functions of B2 symmetry.

There are 248 symmetry adapted basis functions of A1 symmetry.

There are 229 symmetry adapted basis functions of A2 symmetry.

There are 237 symmetry adapted basis functions of B1 symmetry.

There are 240 symmetry adapted basis functions of B2 symmetry.

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

161 alpha electrons 160 beta electrons

nuclear repulsion energy 5370.5691971893 Hartrees.

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

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

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

NAtoms= 78 NActive= 78 NUniq= 21 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=T Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2127821666 Hartrees.

Nuclear repulsion after empirical dispersion term = 5370.3564150227 Hartrees.

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Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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GePol: Number of generator spheres = 78

GePol: Total number of spheres = 78

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

GePol: Number of points = 5762

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.40D-09

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 304

GePol: Fraction of low-weight points (<1% of avg) = 5.28%

GePol: Cavity surface area = 608.558 Ang\*\*2

GePol: Cavity volume = 626.037 Ang\*\*3

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

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PCM non-electrostatic energy = -0.0022048020 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5370.3542102206 Hartrees.

Leave Link 301 at Sun Aug 18 14:21:11 2019, MaxMem= 2013265920 cpu: 1.1

(Enter /home/kira/g09/l302.exe)

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

NBasis= 954 RedAO= T EigKep= 6.36D-05 NBF= 248 229 237 240

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 248 229 237 240

Precomputing XC quadrature grid using

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

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

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

Leave Link 302 at Sun Aug 18 14:21:12 2019, MaxMem= 2013265920 cpu: 10.5

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

DipDrv: MaxL=1.

Leave Link 303 at Sun Aug 18 14:21:12 2019, MaxMem= 2013265920 cpu: 1.4

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

Initial guess from the checkpoint file: "TPPcation.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-A1.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7877 S= 0.5187

Generating alternative initial guess.

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -1914.09100065309

Leave Link 401 at Sun Aug 18 14:21:18 2019, MaxMem= 2013265920 cpu: 44.8

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3049894 IEndB= 3049894 NGot= 2013265920 MDV= 2011237673

LenX= 2011237673 LenY= 2010232667

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

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

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

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

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

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 99601932.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.88D-15 for 5726.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.62D-15 for 3589 345.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.33D-15 for 5726.

Iteration 1 A^-1\*A deviation from orthogonality is 2.73D-12 for 5112 5109.

E= -1914.19841248381

DIIS: error= 2.10D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.19841248381 IErMin= 1 ErrMin= 2.10D-03

ErrMax= 2.10D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.15D-03 BMatP= 5.15D-03

IDIUse=3 WtCom= 9.79D-01 WtEn= 2.10D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.503 Goal= None Shift= 0.000

Gap= 0.515 Goal= None Shift= 0.000

GapD= 0.503 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=4.91D-05 MaxDP=1.61D-03 OVMax= 9.37D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.91D-05 CP: 1.00D+00

E= -1914.20115794054 Delta-E= -0.002745456736 Rises=F Damp=F

DIIS: error= 2.90D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.20115794054 IErMin= 2 ErrMin= 2.90D-04

ErrMax= 2.90D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.60D-05 BMatP= 5.15D-03

IDIUse=3 WtCom= 9.97D-01 WtEn= 2.90D-03

Coeff-Com: -0.694D-01 0.107D+01

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

Coeff: -0.692D-01 0.107D+01

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=9.52D-06 MaxDP=2.36D-04 DE=-2.75D-03 OVMax= 1.48D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 8.70D-06 CP: 1.00D+00 1.08D+00

E= -1914.20120075905 Delta-E= -0.000042818509 Rises=F Damp=F

DIIS: error= 7.18D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.20120075905 IErMin= 3 ErrMin= 7.18D-05

ErrMax= 7.18D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.47D-05 BMatP= 7.60D-05

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

Coeff-Com: -0.325D-01 0.404D+00 0.629D+00

Coeff: -0.325D-01 0.404D+00 0.629D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=4.25D-06 MaxDP=2.24D-04 DE=-4.28D-05 OVMax= 1.06D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 3.57D-06 CP: 1.00D+00 1.09D+00 7.51D-01

E= -1914.20120440999 Delta-E= -0.000003650934 Rises=F Damp=F

DIIS: error= 5.99D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.20120440999 IErMin= 4 ErrMin= 5.99D-05

ErrMax= 5.99D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.14D-05 BMatP= 2.47D-05

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

Coeff-Com: -0.988D-02 0.938D-01 0.403D+00 0.513D+00

Coeff: -0.988D-02 0.938D-01 0.403D+00 0.513D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=1.91D-06 MaxDP=1.23D-04 DE=-3.65D-06 OVMax= 4.21D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.02D-06 CP: 1.00D+00 1.10D+00 8.25D-01 5.92D-01

E= -1914.20120715577 Delta-E= -0.000002745788 Rises=F Damp=F

DIIS: error= 1.08D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.20120715577 IErMin= 5 ErrMin= 1.08D-05

ErrMax= 1.08D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.15D-07 BMatP= 1.14D-05

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

Coeff-Com: -0.228D-03-0.109D-01 0.781D-01 0.182D+00 0.751D+00

Coeff: -0.228D-03-0.109D-01 0.781D-01 0.182D+00 0.751D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=5.12D-07 MaxDP=3.80D-05 DE=-2.75D-06 OVMax= 2.00D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.70D-07 CP: 1.00D+00 1.10D+00 8.42D-01 6.54D-01 7.72D-01

E= -1914.20120720775 Delta-E= -0.000000051977 Rises=F Damp=F

DIIS: error= 7.58D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.20120720775 IErMin= 6 ErrMin= 7.58D-06

ErrMax= 7.58D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.59D-07 BMatP= 3.15D-07

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

Coeff-Com: 0.804D-03-0.162D-01 0.105D-01 0.648D-01 0.485D+00 0.455D+00

Coeff: 0.804D-03-0.162D-01 0.105D-01 0.648D-01 0.485D+00 0.455D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=2.45D-07 MaxDP=1.71D-05 DE=-5.20D-08 OVMax= 5.98D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.24D-07 CP: 1.00D+00 1.10D+00 8.47D-01 6.47D-01 8.48D-01

CP: 4.91D-01

E= -1914.20120724556 Delta-E= -0.000000037810 Rises=F Damp=F

DIIS: error= 1.92D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.20120724556 IErMin= 7 ErrMin= 1.92D-06

ErrMax= 1.92D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.92D-09 BMatP= 1.59D-07

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

Coeff-Com: 0.433D-03-0.785D-02 0.119D-02 0.229D-01 0.216D+00 0.239D+00

Coeff-Com: 0.528D+00

Coeff: 0.433D-03-0.785D-02 0.119D-02 0.229D-01 0.216D+00 0.239D+00

Coeff: 0.528D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=6.40D-08 MaxDP=5.82D-06 DE=-3.78D-08 OVMax= 3.58D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 5.61D-08 CP: 1.00D+00 1.10D+00 8.47D-01 6.52D-01 8.47D-01

CP: 5.36D-01 8.52D-01

E= -1914.20120724807 Delta-E= -0.000000002510 Rises=F Damp=F

DIIS: error= 1.23D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.20120724807 IErMin= 8 ErrMin= 1.23D-06

ErrMax= 1.23D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.53D-09 BMatP= 6.92D-09

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

Coeff-Com: -0.171D-03 0.383D-02-0.370D-02-0.195D-01-0.116D+00-0.105D+00

Coeff-Com: 0.222D+00 0.102D+01

Coeff: -0.171D-03 0.383D-02-0.370D-02-0.195D-01-0.116D+00-0.105D+00

Coeff: 0.222D+00 0.102D+01

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=5.43D-08 MaxDP=5.38D-06 DE=-2.51D-09 OVMax= 2.88D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.32D-08 CP: 1.00D+00 1.10D+00 8.47D-01 6.50D-01 8.59D-01

CP: 5.67D-01 1.20D+00 1.27D+00

E= -1914.20120724966 Delta-E= -0.000000001587 Rises=F Damp=F

DIIS: error= 8.42D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.20120724966 IErMin= 9 ErrMin= 8.42D-07

ErrMax= 8.42D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.29D-10 BMatP= 1.53D-09

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

Coeff-Com: -0.175D-03 0.351D-02-0.188D-02-0.144D-01-0.102D+00-0.104D+00

Coeff-Com: 0.123D-01 0.487D+00 0.720D+00

Coeff: -0.175D-03 0.351D-02-0.188D-02-0.144D-01-0.102D+00-0.104D+00

Coeff: 0.123D-01 0.487D+00 0.720D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=2.48D-08 MaxDP=2.31D-06 DE=-1.59D-09 OVMax= 1.42D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.41D-08 CP: 1.00D+00 1.10D+00 8.48D-01 6.50D-01 8.61D-01

CP: 5.86D-01 1.31D+00 1.50D+00 1.19D+00

E= -1914.20120725010 Delta-E= -0.000000000444 Rises=F Damp=F

DIIS: error= 4.78D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.20120725010 IErMin=10 ErrMin= 4.78D-07

ErrMax= 4.78D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.52D-10 BMatP= 4.29D-10

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

Coeff-Com: 0.142D-05-0.285D-03 0.133D-02 0.352D-02 0.106D-01 0.514D-03

Coeff-Com: -0.111D+00-0.324D+00 0.422D+00 0.998D+00

Coeff: 0.142D-05-0.285D-03 0.133D-02 0.352D-02 0.106D-01 0.514D-03

Coeff: -0.111D+00-0.324D+00 0.422D+00 0.998D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=2.25D-08 MaxDP=1.98D-06 DE=-4.44D-10 OVMax= 1.22D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 5.68D-09 CP: 1.00D+00 1.10D+00 8.48D-01 6.50D-01 8.65D-01

CP: 5.95D-01 1.41D+00 1.70D+00 1.69D+00 1.14D+00

E= -1914.20120725027 Delta-E= -0.000000000164 Rises=F Damp=F

DIIS: error= 1.19D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.20120725027 IErMin=11 ErrMin= 1.19D-07

ErrMax= 1.19D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.75D-11 BMatP= 1.52D-10

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

Coeff-Com: 0.154D-04-0.428D-03 0.767D-03 0.289D-02 0.135D-01 0.872D-02

Coeff-Com: -0.534D-01-0.189D+00 0.141D+00 0.459D+00 0.616D+00

Coeff: 0.154D-04-0.428D-03 0.767D-03 0.289D-02 0.135D-01 0.872D-02

Coeff: -0.534D-01-0.189D+00 0.141D+00 0.459D+00 0.616D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=3.46D-09 MaxDP=2.54D-07 DE=-1.64D-10 OVMax= 1.13D-06

Error on total polarization charges = 0.07903

SCF Done: E(UB3LYP) = -1914.20120725 A.U. after 11 cycles

NFock= 11 Conv=0.35D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7874 S= 0.5185

<L.S>= 0.000000000000E+00

KE= 1.906176114290D+03 PE=-1.515527454213D+04 EE= 5.964543010369D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.38

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7874, after 0.7512

Leave Link 502 at Sun Aug 18 14:25:43 2019, MaxMem= 2013265920 cpu: 2101.4

(Enter /home/kira/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

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

GePol: Maximum number of non-zero 1st derivatives = 188

Leave Link 701 at Sun Aug 18 14:26:00 2019, MaxMem= 2013265920 cpu: 138.0

(Enter /home/kira/g09/l702.exe)

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

Leave Link 702 at Sun Aug 18 14:26:00 2019, MaxMem= 2013265920 cpu: 0.2

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

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

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

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Sun Aug 18 14:26:38 2019, MaxMem= 2013265920 cpu: 305.3

(Enter /home/kira/g09/l716.exe)

Dipole =-2.30296073D-13-1.69819714D-12-2.12632837D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000045214 0.000174429 -0.000000158

2 6 0.000333552 -0.000047237 -0.000109075

3 7 -0.000000000 0.000116219 0.000012688

4 6 -0.000333552 -0.000047237 -0.000109075

5 6 -0.000045214 0.000174429 -0.000000158

6 6 -0.000029610 -0.000100564 0.000070031

7 6 -0.000010880 -0.000295972 0.000170389

8 7 -0.000092095 -0.000000000 -0.000272934

9 6 -0.000010880 0.000295972 0.000170389

10 6 0.000094090 -0.000050933 -0.000039804

11 6 0.000094090 0.000050933 -0.000039804

12 6 0.000029610 -0.000100564 0.000070031

13 6 0.000010880 -0.000295972 0.000170389

14 6 -0.000094090 0.000050933 -0.000039804

15 6 -0.000094090 -0.000050933 -0.000039804

16 6 0.000010880 0.000295972 0.000170389

17 7 0.000092095 0.000000000 -0.000272934

18 6 0.000029610 0.000100564 0.000070031

19 6 0.000333552 0.000047237 -0.000109075

20 6 0.000045214 -0.000174429 -0.000000158

21 6 -0.000045214 -0.000174429 -0.000000158

22 6 -0.000333552 0.000047237 -0.000109075

23 7 -0.000000000 -0.000116219 0.000012688

24 6 -0.000029610 0.000100564 0.000070031

25 6 0.000196623 0.000118828 -0.000017556

26 6 -0.000057744 0.000025208 -0.000006580

27 6 0.000064519 0.000007347 0.000021688

28 6 -0.000020228 -0.000027581 -0.000004992

29 6 -0.000016851 0.000057410 -0.000014796

30 6 -0.000009441 -0.000041948 0.000015298

31 6 0.000020228 -0.000027581 -0.000004992

32 6 -0.000064519 0.000007347 0.000021688

33 6 0.000057744 0.000025208 -0.000006580

34 6 -0.000196623 0.000118828 -0.000017556

35 6 0.000009441 -0.000041948 0.000015298

36 6 0.000016851 0.000057410 -0.000014796

37 6 0.000196623 -0.000118828 -0.000017556

38 6 -0.000009441 0.000041948 0.000015298

39 6 -0.000016851 -0.000057410 -0.000014796

40 6 -0.000020228 0.000027581 -0.000004992

41 6 0.000064519 -0.000007347 0.000021688

42 6 -0.000057744 -0.000025208 -0.000006580

43 6 -0.000196623 -0.000118828 -0.000017556

44 6 0.000009441 0.000041948 0.000015298

45 6 0.000016851 -0.000057410 -0.000014796

46 6 0.000020228 0.000027581 -0.000004992

47 6 -0.000064519 -0.000007347 0.000021688

48 6 0.000057744 -0.000025208 -0.000006580

49 1 0.000019853 -0.000065442 0.000069038

50 1 -0.000019853 -0.000065442 0.000069038

51 1 -0.000069383 0.000046785 -0.000061146

52 1 -0.000069383 -0.000046785 -0.000061146

53 1 0.000069383 -0.000046785 -0.000061146

54 1 0.000069383 0.000046785 -0.000061146

55 1 0.000019853 0.000065442 0.000069038

56 1 -0.000019853 0.000065442 0.000069038

57 1 -0.000074272 -0.000032932 0.000012344

58 1 -0.000004328 0.000015376 -0.000000518

59 1 -0.000004926 -0.000003069 0.000000464

60 1 0.000015356 -0.000007474 0.000002130

61 1 -0.000030626 -0.000062582 -0.000037579

62 1 0.000004926 -0.000003069 0.000000464

63 1 0.000004328 0.000015376 -0.000000518

64 1 0.000074272 -0.000032932 0.000012344

65 1 0.000030626 -0.000062582 -0.000037579

66 1 -0.000015356 -0.000007474 0.000002130

67 1 -0.000030626 0.000062582 -0.000037579

68 1 0.000015356 0.000007474 0.000002130

69 1 -0.000004926 0.000003069 0.000000464

70 1 -0.000004328 -0.000015376 -0.000000518

71 1 -0.000074272 0.000032932 0.000012344

72 1 0.000030626 0.000062582 -0.000037579

73 1 -0.000015356 0.000007474 0.000002130

74 1 0.000004926 0.000003069 0.000000464

75 1 0.000004328 -0.000015376 -0.000000518

76 1 0.000074272 0.000032932 0.000012344

77 1 -0.000000000 -0.000373342 0.000121888

78 1 0.000000000 0.000373342 0.000121888

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

Cartesian Forces: Max 0.000373342 RMS 0.000095329

Leave Link 716 at Sun Aug 18 14:26:38 2019, MaxMem= 2013265920 cpu: 0.2

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

Internal Forces: Max 0.000339853 RMS 0.000074760

Search for a local minimum.

Step number 7 out of a maximum of 452

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

RMS Force = .74760D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 3 4 5 6 7

DE= -8.60D-05 DEPred=-8.18D-05 R= 1.05D+00

TightC=F SS= 1.41D+00 RLast= 5.90D-02 DXNew= 1.3414D+00 1.7707D-01

Trust test= 1.05D+00 RLast= 5.90D-02 DXMaxT set to 7.98D-01

ITU= 1 1 -1 1 1 1 0

Eigenvalues --- 0.00620 0.00861 0.00861 0.00861 0.01579

Eigenvalues --- 0.01654 0.01669 0.01671 0.01686 0.01693

Eigenvalues --- 0.01710 0.01710 0.01710 0.01711 0.01733

Eigenvalues --- 0.01740 0.01745 0.01830 0.01857 0.01869

Eigenvalues --- 0.01908 0.01909 0.01910 0.01910 0.01931

Eigenvalues --- 0.01949 0.02007 0.02010 0.02021 0.02023

Eigenvalues --- 0.02029 0.02041 0.02057 0.02064 0.02074

Eigenvalues --- 0.02079 0.02094 0.02099 0.02099 0.02099

Eigenvalues --- 0.02100 0.02122 0.02132 0.02132 0.02132

Eigenvalues --- 0.02141 0.02141 0.02141 0.02141 0.02161

Eigenvalues --- 0.02161 0.02161 0.02165 0.02165 0.02165

Eigenvalues --- 0.02165 0.02171 0.02171 0.02171 0.02171

Eigenvalues --- 0.02173 0.02175 0.02175 0.02175 0.02176

Eigenvalues --- 0.02176 0.02176 0.02176 0.02212 0.02216

Eigenvalues --- 0.02225 0.02230 0.02231 0.03120 0.03900

Eigenvalues --- 0.15688 0.15985 0.15985 0.15989 0.15989

Eigenvalues --- 0.15992 0.15994 0.15994 0.15994 0.15994

Eigenvalues --- 0.15995 0.15995 0.15995 0.15995 0.15999

Eigenvalues --- 0.15999 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16002 0.16034 0.16223

Eigenvalues --- 0.21998 0.21999 0.21999 0.21999 0.22000

Eigenvalues --- 0.22000 0.22000 0.22012 0.22742 0.22786

Eigenvalues --- 0.22794 0.22799 0.22808 0.23475 0.23475

Eigenvalues --- 0.23475 0.23530 0.23761 0.23862 0.24431

Eigenvalues --- 0.24710 0.24749 0.24781 0.24995 0.24995

Eigenvalues --- 0.24996 0.24998 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25002 0.25089

Eigenvalues --- 0.26127 0.28656 0.32469 0.33146 0.33146

Eigenvalues --- 0.33146 0.34572 0.34601 0.35400 0.35400

Eigenvalues --- 0.35400 0.35400 0.35400 0.35400 0.35400

Eigenvalues --- 0.35404 0.35405 0.35405 0.35405 0.35407

Eigenvalues --- 0.35452 0.35452 0.35452 0.35458 0.35461

Eigenvalues --- 0.35461 0.35461 0.35567 0.36108 0.36108

Eigenvalues --- 0.36108 0.36174 0.36232 0.36232 0.36232

Eigenvalues --- 0.36298 0.36592 0.36873 0.37384 0.37412

Eigenvalues --- 0.38005 0.39522 0.40906 0.41998 0.41998

Eigenvalues --- 0.41998 0.42159 0.42159 0.42159 0.42168

Eigenvalues --- 0.42749 0.43253 0.43494 0.44377 0.44413

Eigenvalues --- 0.44843 0.45318 0.45484 0.45541 0.45632

Eigenvalues --- 0.45852 0.45856 0.45856 0.45856 0.46025

Eigenvalues --- 0.46150 0.46150 0.46150 0.46274 0.46294

Eigenvalues --- 0.46645 0.46645 0.46645 0.46645 0.46834

Eigenvalues --- 0.46834 0.46834 0.47192 0.47585 0.47655

Eigenvalues --- 0.48575 0.48629 0.49741 0.49858 0.50646

Eigenvalues --- 0.52763 0.53080 0.56920

En-DIIS/RFO-DIIS IScMMF= 0 using points: 7 6 5 4 3

RFO step: Lambda=-9.59952788D-06.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 4.72D-04 SmlDif= 1.00D-05

RMS Error= 0.4072814021D-03 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.10035 -0.14531 0.21237 -0.22722 0.05981

Iteration 1 RMS(Cart)= 0.02838383 RMS(Int)= 0.00018246

Iteration 2 RMS(Cart)= 0.00032935 RMS(Int)= 0.00001043

Iteration 3 RMS(Cart)= 0.00000004 RMS(Int)= 0.00001043

ITry= 1 IFail=0 DXMaxC= 1.02D-01 DCOld= 1.00D+10 DXMaxT= 7.98D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.62D-08 for atom 62.

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

(Linear) (Quad) (Total)

R1 2.69495 0.00008 -0.00039 0.00048 0.00008 2.69503

R2 2.59645 -0.00018 0.00097 -0.00074 0.00021 2.59666

R3 2.03629 -0.00005 -0.00001 -0.00003 -0.00004 2.03625

R4 2.59052 -0.00012 -0.00022 -0.00020 -0.00040 2.59012

R5 2.67122 -0.00002 0.00066 -0.00030 0.00036 2.67158

R6 2.59052 -0.00012 -0.00022 -0.00020 -0.00040 2.59012

R7 1.90963 0.00034 -0.00046 0.00059 0.00012 1.90975

R8 2.69495 0.00008 -0.00039 0.00048 0.00008 2.69503

R9 2.67122 -0.00002 0.00066 -0.00030 0.00036 2.67158

R10 2.03629 -0.00005 -0.00001 -0.00003 -0.00004 2.03625

R11 2.66596 -0.00012 0.00030 0.00001 0.00031 2.66627

R12 2.79860 0.00008 -0.00110 0.00024 -0.00086 2.79774

R13 2.58203 -0.00022 0.00001 -0.00054 -0.00052 2.58151

R14 2.74992 0.00001 -0.00015 0.00015 -0.00001 2.74991

R15 2.58203 -0.00022 0.00001 -0.00054 -0.00052 2.58151

R16 2.74992 0.00001 -0.00015 0.00015 -0.00001 2.74991

R17 2.66596 -0.00012 0.00030 0.00001 0.00031 2.66627

R18 2.56192 -0.00012 0.00035 -0.00005 0.00028 2.56221

R19 2.03833 -0.00007 0.00004 -0.00011 -0.00008 2.03825

R20 2.03833 -0.00007 0.00004 -0.00011 -0.00008 2.03825

R21 2.66596 -0.00012 0.00030 0.00001 0.00031 2.66627

R22 2.79860 0.00008 -0.00110 0.00024 -0.00086 2.79774

R23 2.74992 0.00001 -0.00015 0.00015 -0.00001 2.74991

R24 2.58203 -0.00022 0.00001 -0.00054 -0.00052 2.58151

R25 2.56192 -0.00012 0.00035 -0.00005 0.00028 2.56221

R26 2.03833 -0.00007 0.00004 -0.00011 -0.00008 2.03825

R27 2.74992 0.00001 -0.00015 0.00015 -0.00001 2.74991

R28 2.03833 -0.00007 0.00004 -0.00011 -0.00008 2.03825

R29 2.58203 -0.00022 0.00001 -0.00054 -0.00052 2.58151

R30 2.66596 -0.00012 0.00030 0.00001 0.00031 2.66627

R31 2.67122 -0.00002 0.00066 -0.00030 0.00036 2.67158

R32 2.79860 0.00008 -0.00110 0.00024 -0.00086 2.79774

R33 2.69495 0.00008 -0.00039 0.00048 0.00008 2.69503

R34 2.59052 -0.00012 -0.00022 -0.00020 -0.00040 2.59012

R35 2.59645 -0.00018 0.00097 -0.00074 0.00021 2.59666

R36 2.03629 -0.00005 -0.00001 -0.00003 -0.00004 2.03625

R37 2.69495 0.00008 -0.00039 0.00048 0.00008 2.69503

R38 2.03629 -0.00005 -0.00001 -0.00003 -0.00004 2.03625

R39 2.59052 -0.00012 -0.00022 -0.00020 -0.00040 2.59012

R40 2.67122 -0.00002 0.00066 -0.00030 0.00036 2.67158

R41 1.90963 0.00034 -0.00046 0.00059 0.00012 1.90975

R42 2.79860 0.00008 -0.00110 0.00024 -0.00086 2.79774

R43 2.65087 -0.00002 0.00058 -0.00012 0.00046 2.65133

R44 2.65094 -0.00007 0.00057 -0.00020 0.00037 2.65131

R45 2.62821 0.00004 -0.00020 0.00009 -0.00011 2.62810

R46 2.04812 0.00005 -0.00005 0.00007 0.00002 2.04814

R47 2.63515 -0.00000 0.00002 0.00000 0.00003 2.63518

R48 2.04945 0.00001 0.00001 0.00000 0.00001 2.04946

R49 2.63562 0.00000 0.00003 -0.00001 0.00003 2.63564

R50 2.04978 -0.00001 0.00000 -0.00002 -0.00001 2.04976

R51 2.62769 0.00002 -0.00019 0.00005 -0.00014 2.62755

R52 2.04946 0.00001 0.00001 0.00000 0.00001 2.04947

R53 2.04793 0.00002 -0.00008 0.00003 -0.00004 2.04789

R54 2.63515 -0.00000 0.00002 0.00000 0.00003 2.63518

R55 2.63562 0.00000 0.00003 -0.00001 0.00003 2.63564

R56 2.04978 -0.00001 0.00000 -0.00002 -0.00001 2.04976

R57 2.62821 0.00004 -0.00020 0.00009 -0.00011 2.62810

R58 2.04945 0.00001 0.00001 0.00000 0.00001 2.04946

R59 2.65087 -0.00002 0.00058 -0.00012 0.00046 2.65133

R60 2.04812 0.00005 -0.00005 0.00007 0.00002 2.04814

R61 2.65094 -0.00007 0.00057 -0.00020 0.00037 2.65131

R62 2.62769 0.00002 -0.00019 0.00005 -0.00014 2.62755

R63 2.04793 0.00002 -0.00008 0.00003 -0.00004 2.04789

R64 2.04946 0.00001 0.00001 0.00000 0.00001 2.04947

R65 2.65094 -0.00007 0.00057 -0.00020 0.00037 2.65131

R66 2.65087 -0.00002 0.00058 -0.00012 0.00046 2.65133

R67 2.62769 0.00002 -0.00019 0.00005 -0.00014 2.62755

R68 2.04793 0.00002 -0.00008 0.00003 -0.00004 2.04789

R69 2.63562 0.00000 0.00003 -0.00001 0.00003 2.63564

R70 2.04946 0.00001 0.00001 0.00000 0.00001 2.04947

R71 2.63515 -0.00000 0.00002 0.00000 0.00003 2.63518

R72 2.04978 -0.00001 0.00000 -0.00002 -0.00001 2.04976

R73 2.62821 0.00004 -0.00020 0.00009 -0.00011 2.62810

R74 2.04945 0.00001 0.00001 0.00000 0.00001 2.04946

R75 2.04812 0.00005 -0.00005 0.00007 0.00002 2.04814

R76 2.65094 -0.00007 0.00057 -0.00020 0.00037 2.65131

R77 2.65087 -0.00002 0.00058 -0.00012 0.00046 2.65133

R78 2.62769 0.00002 -0.00019 0.00005 -0.00014 2.62755

R79 2.04793 0.00002 -0.00008 0.00003 -0.00004 2.04789

R80 2.63562 0.00000 0.00003 -0.00001 0.00003 2.63564

R81 2.04946 0.00001 0.00001 0.00000 0.00001 2.04947

R82 2.63515 -0.00000 0.00002 0.00000 0.00003 2.63518

R83 2.04978 -0.00001 0.00000 -0.00002 -0.00001 2.04976

R84 2.62821 0.00004 -0.00020 0.00009 -0.00011 2.62810

R85 2.04945 0.00001 0.00001 0.00000 0.00001 2.04946

R86 2.04812 0.00005 -0.00005 0.00007 0.00002 2.04814

A1 1.88325 -0.00008 -0.00014 -0.00009 -0.00023 1.88302

A2 2.18315 0.00002 0.00036 -0.00034 0.00002 2.18317

A3 2.21647 0.00005 -0.00024 0.00042 0.00018 2.21666

A4 1.86580 0.00018 -0.00007 0.00029 0.00022 1.86602

A5 2.21381 -0.00011 0.00118 0.00015 0.00128 2.21509

A6 2.20349 -0.00007 -0.00113 -0.00045 -0.00156 2.20193

A7 1.92607 -0.00021 0.00025 -0.00041 -0.00016 1.92591

A8 2.17854 0.00011 -0.00012 0.00020 0.00009 2.17863

A9 2.17854 0.00011 -0.00012 0.00020 0.00009 2.17863

A10 1.86580 0.00018 -0.00007 0.00029 0.00022 1.86602

A11 2.20349 -0.00007 -0.00113 -0.00045 -0.00156 2.20193

A12 2.21381 -0.00011 0.00118 0.00015 0.00128 2.21509

A13 1.88325 -0.00008 -0.00014 -0.00009 -0.00023 1.88302

A14 2.21647 0.00005 -0.00024 0.00042 0.00018 2.21666

A15 2.18315 0.00002 0.00036 -0.00034 0.00002 2.18317

A16 2.18284 -0.00002 -0.00212 0.00022 -0.00184 2.18099

A17 2.03650 0.00000 0.00082 -0.00006 0.00073 2.03723

A18 2.06384 0.00002 0.00130 -0.00016 0.00111 2.06495

A19 2.18515 -0.00015 -0.00112 -0.00047 -0.00155 2.18360

A20 2.16376 -0.00003 0.00113 0.00009 0.00118 2.16494

A21 1.93410 0.00018 -0.00005 0.00035 0.00031 1.93440

A22 1.84249 -0.00017 -0.00007 -0.00017 -0.00024 1.84225

A23 1.93410 0.00018 -0.00005 0.00035 0.00031 1.93440

A24 2.18515 -0.00015 -0.00112 -0.00047 -0.00155 2.18360

A25 2.16376 -0.00003 0.00113 0.00009 0.00118 2.16494

A26 1.85659 -0.00010 -0.00007 -0.00022 -0.00028 1.85631

A27 2.19989 0.00005 0.00020 -0.00010 0.00010 2.19999

A28 2.22631 0.00004 -0.00014 0.00028 0.00013 2.22644

A29 1.85659 -0.00010 -0.00007 -0.00022 -0.00028 1.85631

A30 2.19989 0.00005 0.00020 -0.00010 0.00010 2.19999

A31 2.22631 0.00004 -0.00014 0.00028 0.00013 2.22644

A32 2.18284 -0.00002 -0.00212 0.00022 -0.00184 2.18099

A33 2.03650 0.00000 0.00082 -0.00006 0.00073 2.03723

A34 2.06384 0.00002 0.00130 -0.00016 0.00111 2.06495

A35 2.16376 -0.00003 0.00113 0.00009 0.00118 2.16494

A36 2.18515 -0.00015 -0.00112 -0.00047 -0.00155 2.18360

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D2 -3.10809 0.00011 0.00482 0.00162 0.00645 -3.10164

D3 -3.09680 0.00007 0.00281 0.00066 0.00347 -3.09333

D4 0.05878 0.00009 0.00536 0.00183 0.00720 0.06599

D5 0.00000 -0.00000 -0.00000 0.00000 -0.00000 0.00000

D6 -3.11569 -0.00002 0.00055 0.00023 0.00077 -3.11492

D7 3.11569 0.00002 -0.00055 -0.00023 -0.00077 3.11492

D8 0.00000 0.00000 0.00000 0.00000 -0.00000 0.00000

D9 -0.03251 -0.00013 -0.00377 -0.00075 -0.00453 -0.03704

D10 3.09965 -0.00007 -0.00068 -0.00162 -0.00231 3.09735

D11 3.09519 -0.00016 -0.00630 -0.00190 -0.00820 3.08700

D12 -0.05583 -0.00009 -0.00321 -0.00277 -0.00597 -0.06180

D13 -2.98075 -0.00000 0.00896 -0.00195 0.00701 -2.97374

D14 0.15518 0.00003 0.00953 -0.00166 0.00788 0.16306

D15 0.17745 0.00002 0.01198 -0.00057 0.01141 0.18886

D16 -2.96981 0.00006 0.01255 -0.00028 0.01228 -2.95753

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D29 -0.17069 -0.00007 -0.00989 -0.00255 -0.01245 -0.18314

D30 2.99273 -0.00009 -0.00746 -0.00078 -0.00823 2.98449

D31 2.96515 -0.00004 -0.00932 -0.00225 -0.01157 2.95359

D32 -0.15461 -0.00005 -0.00688 -0.00047 -0.00735 -0.16197

D33 -0.98128 0.00012 0.01299 0.00092 0.01391 -0.96737

D34 2.16031 0.00011 0.01287 0.00014 0.01301 2.17332

D35 2.16558 0.00008 0.01247 0.00064 0.01311 2.17869

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D37 -3.08272 0.00013 0.00790 -0.00044 0.00746 -3.07526

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D41 -0.02490 -0.00009 -0.00363 0.00127 -0.00236 -0.02726

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D55 3.11222 0.00002 -0.00015 -0.00139 -0.00154 3.11068

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D91 2.16031 0.00011 0.01287 0.00014 0.01301 2.17332

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D99 0.03251 0.00013 0.00377 0.00075 0.00453 0.03704

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D103 -3.11569 -0.00002 0.00055 0.00023 0.00077 -3.11492

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D164 -3.12298 -0.00002 0.00109 -0.00005 0.00105 -3.12193

D165 0.01791 -0.00000 -0.00022 0.00037 0.00015 0.01807

D166 -3.12348 -0.00001 0.00018 -0.00012 0.00005 -3.12343

D167 3.13223 0.00002 -0.00113 0.00039 -0.00073 3.13150

D168 -0.00917 0.00001 -0.00073 -0.00010 -0.00083 -0.01000

D169 3.13308 -0.00001 0.00007 -0.00079 -0.00072 3.13236

D170 0.01862 -0.00003 0.00097 -0.00082 0.00015 0.01877

D171 -0.00852 0.00000 0.00019 -0.00002 0.00017 -0.00834

D172 -3.12298 -0.00002 0.00109 -0.00005 0.00105 -3.12193

D173 3.13198 0.00001 0.00013 0.00034 0.00047 3.13244

D174 0.01853 -0.00001 0.00095 0.00030 0.00125 0.01978

D175 -0.00961 -0.00000 0.00001 -0.00044 -0.00043 -0.01004

D176 -3.12306 -0.00002 0.00082 -0.00047 0.00035 -3.12271

D177 0.01791 -0.00000 -0.00022 0.00037 0.00015 0.01807

D178 -3.12348 -0.00001 0.00018 -0.00012 0.00005 -3.12343

D179 3.13223 0.00002 -0.00113 0.00039 -0.00073 3.13150

D180 -0.00917 0.00001 -0.00073 -0.00010 -0.00083 -0.01000

D181 -0.00916 -0.00000 0.00004 -0.00026 -0.00022 -0.00938

D182 3.13253 -0.00000 0.00010 -0.00018 -0.00008 3.13245

D183 3.13224 0.00001 -0.00036 0.00023 -0.00012 3.13212

D184 -0.00926 0.00001 -0.00030 0.00032 0.00002 -0.00924

D185 -0.00898 0.00000 0.00016 -0.00020 -0.00003 -0.00901

D186 3.13249 0.00001 -0.00021 0.00036 0.00015 3.13264

D187 3.13252 -0.00000 0.00010 -0.00028 -0.00018 3.13235

D188 -0.00919 0.00001 -0.00027 0.00028 0.00000 -0.00919

D189 0.01838 0.00000 -0.00018 0.00055 0.00036 0.01874

D190 3.13170 0.00002 -0.00101 0.00058 -0.00043 3.13127

D191 -3.12309 -0.00001 0.00019 -0.00001 0.00018 -3.12291

D192 -0.00977 0.00001 -0.00063 0.00002 -0.00061 -0.01038

D193 -3.13308 0.00001 -0.00007 0.00079 0.00072 -3.13236

D194 -0.01862 0.00003 -0.00097 0.00082 -0.00015 -0.01877

D195 0.00852 -0.00000 -0.00019 0.00002 -0.00017 0.00834

D196 3.12298 0.00002 -0.00109 0.00005 -0.00105 3.12193

D197 -3.13198 -0.00001 -0.00013 -0.00034 -0.00047 -3.13244

D198 -0.01853 0.00001 -0.00095 -0.00030 -0.00125 -0.01978

D199 0.00961 0.00000 -0.00001 0.00044 0.00043 0.01004

D200 3.12306 0.00002 -0.00082 0.00047 -0.00035 3.12271

D201 -0.01791 0.00000 0.00022 -0.00037 -0.00015 -0.01807

D202 3.12348 0.00001 -0.00018 0.00012 -0.00005 3.12343

D203 -3.13223 -0.00002 0.00113 -0.00039 0.00073 -3.13150

D204 0.00917 -0.00001 0.00073 0.00010 0.00083 0.01000

D205 0.00916 0.00000 -0.00004 0.00026 0.00022 0.00938

D206 -3.13253 0.00000 -0.00010 0.00018 0.00008 -3.13245

D207 -3.13224 -0.00001 0.00036 -0.00023 0.00012 -3.13212

D208 0.00926 -0.00001 0.00030 -0.00032 -0.00002 0.00924

D209 0.00898 -0.00000 -0.00016 0.00020 0.00003 0.00901

D210 -3.13249 -0.00001 0.00021 -0.00036 -0.00015 -3.13264

D211 -3.13252 0.00000 -0.00010 0.00028 0.00018 -3.13235

D212 0.00919 -0.00001 0.00027 -0.00028 -0.00000 0.00919

D213 -0.01838 -0.00000 0.00018 -0.00055 -0.00036 -0.01874

D214 -3.13170 -0.00002 0.00101 -0.00058 0.00043 -3.13127

D215 3.12309 0.00001 -0.00019 0.00001 -0.00018 3.12291

D216 0.00977 -0.00001 0.00063 -0.00002 0.00061 0.01038

Item Value Threshold Converged?

Maximum Force 0.000340 0.000450 YES

RMS Force 0.000075 0.000300 YES

Maximum Displacement 0.102119 0.001800 NO

RMS Displacement 0.028430 0.001200 NO

Predicted change in Energy=-3.600573D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Aug 18 14:26:38 2019, MaxMem= 2013265920 cpu: 1.5

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

Stoichiometry C44H30N4(1+,2)

Framework group C2V[SGV(H2N2),SGV'(N2),X(C44H28)]

Deg. of freedom 59

Full point group C2V NOp 4

RotChk: IX=0 Diff= 6.07D-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 -0.687046 4.172673 0.512934

2 6 0 -1.125129 2.863551 0.154915

3 7 0 0.000000 2.101349 -0.023320

4 6 0 1.125129 2.863551 0.154915

5 6 0 0.687046 4.172673 0.512934

6 6 0 2.460780 2.430642 -0.010282

7 6 0 2.860833 1.087784 -0.175828

8 7 0 2.053436 -0.000000 0.000245

9 6 0 2.860833 -1.087784 -0.175828

10 6 0 4.211313 -0.677930 -0.530516

11 6 0 4.211313 0.677930 -0.530516

12 6 0 -2.460780 2.430642 -0.010282

13 6 0 -2.860833 1.087784 -0.175828

14 6 0 -4.211313 0.677930 -0.530516

15 6 0 -4.211313 -0.677930 -0.530516

16 6 0 -2.860833 -1.087784 -0.175828

17 7 0 -2.053436 0.000000 0.000245

18 6 0 -2.460780 -2.430642 -0.010282

19 6 0 -1.125129 -2.863551 0.154915

20 6 0 -0.687046 -4.172673 0.512934

21 6 0 0.687046 -4.172673 0.512934

22 6 0 1.125129 -2.863551 0.154915

23 7 0 -0.000000 -2.101349 -0.023320

24 6 0 2.460780 -2.430642 -0.010282

25 6 0 3.506401 3.478713 -0.000517

26 6 0 3.439802 4.562339 -0.889220

27 6 0 4.430771 5.538079 -0.882737

28 6 0 5.487232 5.457534 0.023884

29 6 0 5.555240 4.389866 0.918710

30 6 0 4.578483 3.400446 0.901124

31 6 0 -5.487232 5.457534 0.023884

32 6 0 -4.430771 5.538079 -0.882737

33 6 0 -3.439802 4.562339 -0.889220

34 6 0 -3.506401 3.478713 -0.000517

35 6 0 -4.578483 3.400446 0.901124

36 6 0 -5.555240 4.389866 0.918710

37 6 0 3.506401 -3.478713 -0.000517

38 6 0 4.578483 -3.400446 0.901124

39 6 0 5.555240 -4.389866 0.918710

40 6 0 5.487232 -5.457534 0.023884

41 6 0 4.430771 -5.538079 -0.882737

42 6 0 3.439802 -4.562339 -0.889220

43 6 0 -3.506401 -3.478713 -0.000517

44 6 0 -4.578483 -3.400446 0.901124

45 6 0 -5.555240 -4.389866 0.918710

46 6 0 -5.487232 -5.457534 0.023884

47 6 0 -4.430771 -5.538079 -0.882737

48 6 0 -3.439802 -4.562339 -0.889220

49 1 0 -1.335599 4.996344 0.761986

50 1 0 1.335599 4.996344 0.761986

51 1 0 5.031117 -1.335519 -0.773147

52 1 0 5.031117 1.335519 -0.773147

53 1 0 -5.031117 1.335519 -0.773147

54 1 0 -5.031117 -1.335519 -0.773147

55 1 0 -1.335599 -4.996344 0.761986

56 1 0 1.335599 -4.996344 0.761986

57 1 0 2.624544 4.621361 -1.600951

58 1 0 4.377802 6.361847 -1.586156

59 1 0 6.254684 6.224004 0.033332

60 1 0 6.370121 4.327382 1.631645

61 1 0 4.627128 2.576240 1.603059

62 1 0 -6.254684 6.224004 0.033332

63 1 0 -4.377802 6.361847 -1.586156

64 1 0 -2.624544 4.621361 -1.600951

65 1 0 -4.627128 2.576240 1.603059

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67 1 0 4.627128 -2.576240 1.603059

68 1 0 6.370121 -4.327382 1.631645

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71 1 0 2.624544 -4.621361 -1.600951

72 1 0 -4.627128 -2.576240 1.603059

73 1 0 -6.370121 -4.327382 1.631645

74 1 0 -6.254684 -6.224004 0.033332

75 1 0 -4.377802 -6.361847 -1.586156

76 1 0 -2.624544 -4.621361 -1.600951

77 1 0 0.000000 1.115956 -0.247608

78 1 0 -0.000000 -1.115956 -0.247608

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

Rotational constants (GHZ): 0.0592791 0.0586185 0.0302864

Leave Link 202 at Sun Aug 18 14:26:39 2019, MaxMem= 2013265920 cpu: 0.1

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

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

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

There are 261 symmetry adapted cartesian basis functions of A1 symmetry.

There are 240 symmetry adapted cartesian basis functions of A2 symmetry.

There are 249 symmetry adapted cartesian basis functions of B1 symmetry.

There are 252 symmetry adapted cartesian basis functions of B2 symmetry.

There are 248 symmetry adapted basis functions of A1 symmetry.

There are 229 symmetry adapted basis functions of A2 symmetry.

There are 237 symmetry adapted basis functions of B1 symmetry.

There are 240 symmetry adapted basis functions of B2 symmetry.

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

161 alpha electrons 160 beta electrons

nuclear repulsion energy 5372.0195536235 Hartrees.

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

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

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

NAtoms= 78 NActive= 78 NUniq= 21 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=T Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2128188732 Hartrees.

Nuclear repulsion after empirical dispersion term = 5371.8067347503 Hartrees.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 78

GePol: Total number of spheres = 78

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

GePol: Number of points = 5702

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.20D-08

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 290

GePol: Fraction of low-weight points (<1% of avg) = 5.09%

GePol: Cavity surface area = 608.658 Ang\*\*2

GePol: Cavity volume = 626.285 Ang\*\*3

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

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PCM non-electrostatic energy = -0.0022203927 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5371.8045143576 Hartrees.

Leave Link 301 at Sun Aug 18 14:26:39 2019, MaxMem= 2013265920 cpu: 1.1

(Enter /home/kira/g09/l302.exe)

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

NBasis= 954 RedAO= T EigKep= 6.37D-05 NBF= 248 229 237 240

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 248 229 237 240

Precomputing XC quadrature grid using

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

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

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

Leave Link 302 at Sun Aug 18 14:26:40 2019, MaxMem= 2013265920 cpu: 10.4

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

DipDrv: MaxL=1.

Leave Link 303 at Sun Aug 18 14:26:40 2019, MaxMem= 2013265920 cpu: 1.5

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

Initial guess from the checkpoint file: "TPPcation.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) (B1) (A1) (B2) (A2) (A1) (B1) (A2) (B2)

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The electronic state of the initial guess is 2-A1.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7874 S= 0.5185

Generating alternative initial guess.

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -1914.09083143631

Leave Link 401 at Sun Aug 18 14:26:46 2019, MaxMem= 2013265920 cpu: 45.4

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3049894 IEndB= 3049894 NGot= 2013265920 MDV= 2011237673

LenX= 2011237673 LenY= 2010232667

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

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

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

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

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

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 97538412.

Iteration 1 A\*A^-1 deviation from unit magnitude is 9.77D-15 for 5687.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.33D-15 for 5680 4637.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.33D-15 for 5687.

Iteration 1 A^-1\*A deviation from orthogonality is 7.31D-13 for 4219 4214.

E= -1914.19522173470

DIIS: error= 2.83D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.19522173470 IErMin= 1 ErrMin= 2.83D-03

ErrMax= 2.83D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.11D-02 BMatP= 1.11D-02

IDIUse=3 WtCom= 9.72D-01 WtEn= 2.83D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.503 Goal= None Shift= 0.000

Gap= 0.515 Goal= None Shift= 0.000

GapD= 0.503 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=7.23D-05 MaxDP=2.11D-03 OVMax= 1.24D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 7.22D-05 CP: 1.00D+00

E= -1914.20113498444 Delta-E= -0.005913249742 Rises=F Damp=F

DIIS: error= 3.89D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.20113498444 IErMin= 2 ErrMin= 3.89D-04

ErrMax= 3.89D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.58D-04 BMatP= 1.11D-02

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.89D-03

Coeff-Com: -0.713D-01 0.107D+01

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

Coeff: -0.710D-01 0.107D+01

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=1.34D-05 MaxDP=3.31D-04 DE=-5.91D-03 OVMax= 1.94D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.18D-05 CP: 1.00D+00 1.09D+00

E= -1914.20123311372 Delta-E= -0.000098129281 Rises=F Damp=F

DIIS: error= 5.87D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.20123311372 IErMin= 3 ErrMin= 5.87D-05

ErrMax= 5.87D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.98D-05 BMatP= 1.58D-04

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

Coeff-Com: -0.235D-01 0.271D+00 0.753D+00

Coeff: -0.235D-01 0.271D+00 0.753D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=3.84D-06 MaxDP=1.19D-04 DE=-9.81D-05 OVMax= 8.06D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 3.28D-06 CP: 1.00D+00 1.11D+00 8.65D-01

E= -1914.20123714653 Delta-E= -0.000004032805 Rises=F Damp=F

DIIS: error= 4.23D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.20123714653 IErMin= 4 ErrMin= 4.23D-05

ErrMax= 4.23D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.70D-06 BMatP= 1.98D-05

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

Coeff-Com: -0.664D-02 0.570D-01 0.373D+00 0.576D+00

Coeff: -0.664D-02 0.570D-01 0.373D+00 0.576D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=1.58D-06 MaxDP=7.48D-05 DE=-4.03D-06 OVMax= 3.60D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.19D-06 CP: 1.00D+00 1.11D+00 9.06D-01 7.26D-01

E= -1914.20123880556 Delta-E= -0.000001659033 Rises=F Damp=F

DIIS: error= 1.90D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.20123880556 IErMin= 5 ErrMin= 1.90D-05

ErrMax= 1.90D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.42D-07 BMatP= 6.70D-06

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

Coeff-Com: 0.525D-03-0.178D-01 0.568D-01 0.274D+00 0.686D+00

Coeff: 0.525D-03-0.178D-01 0.568D-01 0.274D+00 0.686D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=5.98D-07 MaxDP=3.68D-05 DE=-1.66D-06 OVMax= 2.09D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.95D-07 CP: 1.00D+00 1.11D+00 9.24D-01 7.94D-01 7.29D-01

E= -1914.20123897781 Delta-E= -0.000000172252 Rises=F Damp=F

DIIS: error= 7.89D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.20123897781 IErMin= 6 ErrMin= 7.89D-06

ErrMax= 7.89D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.70D-07 BMatP= 7.42D-07

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

Coeff-Com: 0.801D-03-0.153D-01 0.753D-02 0.128D+00 0.427D+00 0.452D+00

Coeff: 0.801D-03-0.153D-01 0.753D-02 0.128D+00 0.427D+00 0.452D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=2.21D-07 MaxDP=1.38D-05 DE=-1.72D-07 OVMax= 5.15D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.48D-07 CP: 1.00D+00 1.11D+00 9.27D-01 8.00D-01 7.74D-01

CP: 6.20D-01

E= -1914.20123902225 Delta-E= -0.000000044438 Rises=F Damp=F

DIIS: error= 1.77D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.20123902225 IErMin= 7 ErrMin= 1.77D-06

ErrMax= 1.77D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.59D-09 BMatP= 1.70D-07

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

Coeff-Com: 0.165D-03-0.242D-02-0.263D-02 0.101D-01 0.576D-01 0.111D+00

Coeff-Com: 0.826D+00

Coeff: 0.165D-03-0.242D-02-0.263D-02 0.101D-01 0.576D-01 0.111D+00

Coeff: 0.826D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=8.52D-08 MaxDP=9.73D-06 DE=-4.44D-08 OVMax= 5.30D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 6.52D-08 CP: 1.00D+00 1.11D+00 9.28D-01 8.06D-01 7.76D-01

CP: 7.14D-01 1.22D+00

E= -1914.20123902552 Delta-E= -0.000000003271 Rises=F Damp=F

DIIS: error= 1.44D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.20123902552 IErMin= 8 ErrMin= 1.44D-06

ErrMax= 1.44D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.10D-09 BMatP= 4.59D-09

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

Coeff-Com: -0.200D-03 0.435D-02-0.479D-02-0.441D-01-0.129D+00-0.104D+00

Coeff-Com: 0.595D+00 0.682D+00

Coeff: -0.200D-03 0.435D-02-0.479D-02-0.441D-01-0.129D+00-0.104D+00

Coeff: 0.595D+00 0.682D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=6.78D-08 MaxDP=6.74D-06 DE=-3.27D-09 OVMax= 3.31D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 3.32D-08 CP: 1.00D+00 1.11D+00 9.28D-01 8.06D-01 7.93D-01

CP: 7.78D-01 1.54D+00 8.09D-01

E= -1914.20123902791 Delta-E= -0.000000002393 Rises=F Damp=F

DIIS: error= 9.12D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.20123902791 IErMin= 9 ErrMin= 9.12D-07

ErrMax= 9.12D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.26D-10 BMatP= 4.10D-09

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

Coeff-Com: -0.113D-03 0.220D-02-0.117D-02-0.195D-01-0.628D-01-0.653D-01

Coeff-Com: 0.888D-01 0.271D+00 0.787D+00

Coeff: -0.113D-03 0.220D-02-0.117D-02-0.195D-01-0.628D-01-0.653D-01

Coeff: 0.888D-01 0.271D+00 0.787D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=3.12D-08 MaxDP=3.46D-06 DE=-2.39D-09 OVMax= 1.94D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.74D-08 CP: 1.00D+00 1.11D+00 9.29D-01 8.07D-01 7.95D-01

CP: 8.08D-01 1.64D+00 1.07D+00 1.13D+00

E= -1914.20123902838 Delta-E= -0.000000000465 Rises=F Damp=F

DIIS: error= 5.85D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.20123902838 IErMin=10 ErrMin= 5.85D-07

ErrMax= 5.85D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.55D-10 BMatP= 5.26D-10

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

Coeff-Com: 0.123D-04-0.465D-03 0.155D-02 0.667D-02 0.151D-01 0.107D-02

Coeff-Com: -0.214D+00-0.135D+00 0.587D+00 0.738D+00

Coeff: 0.123D-04-0.465D-03 0.155D-02 0.667D-02 0.151D-01 0.107D-02

Coeff: -0.214D+00-0.135D+00 0.587D+00 0.738D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=2.26D-08 MaxDP=2.12D-06 DE=-4.65D-10 OVMax= 8.57D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 9.26D-09 CP: 1.00D+00 1.11D+00 9.29D-01 8.07D-01 7.99D-01

CP: 8.19D-01 1.73D+00 1.13D+00 1.55D+00 9.51D-01

E= -1914.20123902861 Delta-E= -0.000000000235 Rises=F Damp=F

DIIS: error= 1.97D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.20123902861 IErMin=11 ErrMin= 1.97D-07

ErrMax= 1.97D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.56D-11 BMatP= 3.55D-10

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

Coeff-Com: 0.222D-04-0.523D-03 0.755D-03 0.559D-02 0.156D-01 0.107D-01

Coeff-Com: -0.969D-01-0.975D-01 0.110D+00 0.281D+00 0.771D+00

Coeff: 0.222D-04-0.523D-03 0.755D-03 0.559D-02 0.156D-01 0.107D-01

Coeff: -0.969D-01-0.975D-01 0.110D+00 0.281D+00 0.771D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=7.20D-09 MaxDP=4.06D-07 DE=-2.35D-10 OVMax= 2.78D-06

Error on total polarization charges = 0.07902

SCF Done: E(UB3LYP) = -1914.20123903 A.U. after 11 cycles

NFock= 11 Conv=0.72D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7873 S= 0.5185

<L.S>= 0.000000000000E+00

KE= 1.906179317435D+03 PE=-1.515820042544D+04 EE= 5.966015354621D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.39

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7873, after 0.7512

Leave Link 502 at Sun Aug 18 14:31:10 2019, MaxMem= 2013265920 cpu: 2098.9

(Enter /home/kira/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

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

GePol: Maximum number of non-zero 1st derivatives = 184

Leave Link 701 at Sun Aug 18 14:31:28 2019, MaxMem= 2013265920 cpu: 137.8

(Enter /home/kira/g09/l702.exe)

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

Leave Link 702 at Sun Aug 18 14:31:28 2019, MaxMem= 2013265920 cpu: 0.2

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

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

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

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Sun Aug 18 14:32:06 2019, MaxMem= 2013265920 cpu: 308.3

(Enter /home/kira/g09/l716.exe)

Dipole = 1.73824711D-13 2.85815815D-12-2.21649511D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000045781 0.000044737 -0.000037136

2 6 0.000100956 -0.000039046 0.000105147

3 7 -0.000000000 0.000171219 -0.000095039

4 6 -0.000100956 -0.000039046 0.000105147

5 6 -0.000045781 0.000044737 -0.000037136

6 6 -0.000024403 -0.000037951 0.000020583

7 6 0.000058681 -0.000041772 0.000051134

8 7 0.000011682 -0.000000000 -0.000145065

9 6 0.000058681 0.000041772 0.000051134

10 6 -0.000011839 -0.000028024 -0.000031891

11 6 -0.000011839 0.000028024 -0.000031891

12 6 0.000024403 -0.000037951 0.000020583

13 6 -0.000058681 -0.000041772 0.000051134

14 6 0.000011839 0.000028024 -0.000031891

15 6 0.000011839 -0.000028024 -0.000031891

16 6 -0.000058681 0.000041772 0.000051134

17 7 -0.000011682 -0.000000000 -0.000145065

18 6 0.000024403 0.000037951 0.000020583

19 6 0.000100956 0.000039046 0.000105147

20 6 0.000045781 -0.000044737 -0.000037136

21 6 -0.000045781 -0.000044737 -0.000037136

22 6 -0.000100956 0.000039046 0.000105147

23 7 -0.000000000 -0.000171219 -0.000095039

24 6 -0.000024403 0.000037951 0.000020583

25 6 0.000104509 0.000096241 0.000008911

26 6 -0.000047070 -0.000029547 -0.000024778

27 6 0.000018059 0.000004733 0.000015649

28 6 -0.000020825 -0.000017337 0.000004047

29 6 0.000004797 0.000027169 -0.000017670

30 6 -0.000037749 -0.000075704 0.000013514

31 6 0.000020825 -0.000017337 0.000004047

32 6 -0.000018059 0.000004733 0.000015649

33 6 0.000047070 -0.000029547 -0.000024778

34 6 -0.000104509 0.000096241 0.000008911

35 6 0.000037749 -0.000075704 0.000013514

36 6 -0.000004797 0.000027169 -0.000017670

37 6 0.000104509 -0.000096241 0.000008911

38 6 -0.000037749 0.000075704 0.000013514

39 6 0.000004797 -0.000027169 -0.000017670

40 6 -0.000020825 0.000017337 0.000004047

41 6 0.000018059 -0.000004733 0.000015649

42 6 -0.000047070 0.000029547 -0.000024778

43 6 -0.000104509 -0.000096241 0.000008911

44 6 0.000037749 0.000075704 0.000013514

45 6 -0.000004797 -0.000027169 -0.000017670

46 6 0.000020825 0.000017337 0.000004047

47 6 -0.000018059 -0.000004733 0.000015649

48 6 0.000047070 0.000029547 -0.000024778

49 1 -0.000015592 -0.000025786 -0.000002408

50 1 0.000015592 -0.000025786 -0.000002408

51 1 -0.000014027 -0.000012071 0.000004811

52 1 -0.000014027 0.000012071 0.000004811

53 1 0.000014027 0.000012071 0.000004811

54 1 0.000014027 -0.000012071 0.000004811

55 1 -0.000015592 0.000025786 -0.000002408

56 1 0.000015592 0.000025786 -0.000002408

57 1 0.000007550 0.000000655 -0.000002516

58 1 0.000002285 -0.000003283 -0.000004173

59 1 -0.000001744 -0.000001516 -0.000000478

60 1 -0.000002611 0.000000325 0.000002850

61 1 -0.000002226 -0.000006822 -0.000004360

62 1 0.000001744 -0.000001516 -0.000000478

63 1 -0.000002285 -0.000003283 -0.000004173

64 1 -0.000007550 0.000000655 -0.000002516

65 1 0.000002226 -0.000006822 -0.000004360

66 1 0.000002611 0.000000325 0.000002850

67 1 -0.000002226 0.000006822 -0.000004360

68 1 -0.000002611 -0.000000325 0.000002850

69 1 -0.000001744 0.000001516 -0.000000478

70 1 0.000002285 0.000003283 -0.000004173

71 1 0.000007550 -0.000000655 -0.000002516

72 1 0.000002226 0.000006822 -0.000004360

73 1 0.000002611 -0.000000325 0.000002850

74 1 0.000001744 0.000001516 -0.000000478

75 1 -0.000002285 0.000003283 -0.000004173

76 1 -0.000007550 -0.000000655 -0.000002516

77 1 -0.000000000 -0.000150081 0.000037635

78 1 0.000000000 0.000150081 0.000037635

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

Cartesian Forces: Max 0.000171219 RMS 0.000044794

Leave Link 716 at Sun Aug 18 14:32:06 2019, MaxMem= 2013265920 cpu: 0.2

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

Internal Forces: Max 0.000137986 RMS 0.000024335

Search for a local minimum.

Step number 8 out of a maximum of 452

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

RMS Force = .24335D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 3 4 5 6 7

8

DE= -3.18D-05 DEPred=-3.60D-05 R= 8.83D-01

TightC=F SS= 1.41D+00 RLast= 8.80D-02 DXNew= 1.3414D+00 2.6407D-01

Trust test= 8.83D-01 RLast= 8.80D-02 DXMaxT set to 7.98D-01

ITU= 1 1 1 -1 1 1 1 0

Eigenvalues --- 0.00687 0.00861 0.00861 0.00861 0.01551

Eigenvalues --- 0.01653 0.01669 0.01671 0.01685 0.01692

Eigenvalues --- 0.01710 0.01710 0.01710 0.01715 0.01733

Eigenvalues --- 0.01744 0.01773 0.01830 0.01857 0.01869

Eigenvalues --- 0.01884 0.01909 0.01910 0.01912 0.01918

Eigenvalues --- 0.01950 0.01999 0.02007 0.02013 0.02021

Eigenvalues --- 0.02031 0.02042 0.02057 0.02070 0.02081

Eigenvalues --- 0.02096 0.02098 0.02099 0.02099 0.02099

Eigenvalues --- 0.02113 0.02132 0.02132 0.02132 0.02141

Eigenvalues --- 0.02141 0.02141 0.02141 0.02149 0.02161

Eigenvalues --- 0.02161 0.02161 0.02165 0.02165 0.02165

Eigenvalues --- 0.02165 0.02171 0.02171 0.02171 0.02171

Eigenvalues --- 0.02174 0.02175 0.02175 0.02175 0.02176

Eigenvalues --- 0.02176 0.02176 0.02176 0.02212 0.02217

Eigenvalues --- 0.02219 0.02225 0.02233 0.03035 0.03872

Eigenvalues --- 0.15639 0.15984 0.15984 0.15988 0.15988

Eigenvalues --- 0.15991 0.15993 0.15993 0.15993 0.15994

Eigenvalues --- 0.15994 0.15994 0.15994 0.15995 0.15999

Eigenvalues --- 0.15999 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16003 0.16037 0.16200

Eigenvalues --- 0.21999 0.21999 0.21999 0.21999 0.22000

Eigenvalues --- 0.22000 0.22000 0.22011 0.22720 0.22783

Eigenvalues --- 0.22792 0.22796 0.23149 0.23474 0.23474

Eigenvalues --- 0.23474 0.23529 0.23643 0.23811 0.24398

Eigenvalues --- 0.24696 0.24724 0.24767 0.24993 0.24993

Eigenvalues --- 0.24993 0.24997 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25118

Eigenvalues --- 0.26224 0.28350 0.32563 0.33146 0.33146

Eigenvalues --- 0.33146 0.34569 0.34598 0.35400 0.35400

Eigenvalues --- 0.35400 0.35400 0.35400 0.35400 0.35400

Eigenvalues --- 0.35404 0.35405 0.35405 0.35405 0.35413

Eigenvalues --- 0.35452 0.35452 0.35452 0.35458 0.35461

Eigenvalues --- 0.35461 0.35461 0.35561 0.36108 0.36108

Eigenvalues --- 0.36108 0.36167 0.36232 0.36232 0.36232

Eigenvalues --- 0.36308 0.36723 0.36873 0.37380 0.37408

Eigenvalues --- 0.38166 0.39522 0.41095 0.41998 0.41998

Eigenvalues --- 0.41998 0.42159 0.42159 0.42159 0.42169

Eigenvalues --- 0.42731 0.43248 0.43482 0.44372 0.44412

Eigenvalues --- 0.44851 0.45309 0.45484 0.45537 0.45632

Eigenvalues --- 0.45849 0.45856 0.45856 0.45856 0.46034

Eigenvalues --- 0.46150 0.46150 0.46150 0.46271 0.46345

Eigenvalues --- 0.46645 0.46645 0.46645 0.46645 0.46834

Eigenvalues --- 0.46834 0.46834 0.46996 0.47535 0.47769

Eigenvalues --- 0.48570 0.48626 0.49735 0.49854 0.50644

Eigenvalues --- 0.52801 0.53076 0.55693

En-DIIS/RFO-DIIS IScMMF= 0 using points: 8 7 6 5 4

RFO step: Lambda=-6.83437013D-07.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= -7.25D-05 SmlDif= 1.00D-05

RMS Error= 0.8129600151D-04 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 0.94408 0.11261 -0.06739 -0.00071 0.01141

Iteration 1 RMS(Cart)= 0.00238191 RMS(Int)= 0.00000152

Iteration 2 RMS(Cart)= 0.00000213 RMS(Int)= 0.00000125

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000125

ITry= 1 IFail=0 DXMaxC= 8.79D-03 DCOld= 1.00D+10 DXMaxT= 7.98D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 8.23D-09 for atom 54.

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

(Linear) (Quad) (Total)

R1 2.69503 0.00000 0.00005 0.00005 0.00010 2.69513

R2 2.59666 -0.00004 -0.00007 -0.00008 -0.00015 2.59651

R3 2.03625 -0.00001 0.00001 -0.00003 -0.00002 2.03623

R4 2.59012 -0.00004 0.00002 -0.00005 -0.00002 2.59010

R5 2.67158 0.00004 -0.00010 0.00002 -0.00009 2.67150

R6 2.59012 -0.00004 0.00002 -0.00005 -0.00002 2.59010

R7 1.90975 0.00014 -0.00004 0.00035 0.00031 1.91007

R8 2.69503 0.00000 0.00005 0.00005 0.00010 2.69513

R9 2.67158 0.00004 -0.00010 0.00002 -0.00009 2.67150

R10 2.03625 -0.00001 0.00001 -0.00003 -0.00002 2.03623

R11 2.66627 -0.00003 -0.00000 -0.00011 -0.00011 2.66615

R12 2.79774 0.00001 0.00006 0.00011 0.00017 2.79791

R13 2.58151 -0.00007 0.00001 -0.00016 -0.00015 2.58136

R14 2.74991 -0.00002 0.00002 -0.00003 -0.00002 2.74990

R15 2.58151 -0.00007 0.00001 -0.00016 -0.00015 2.58136

R16 2.74991 -0.00002 0.00002 -0.00003 -0.00002 2.74990

R17 2.66627 -0.00003 -0.00000 -0.00011 -0.00011 2.66615

R18 2.56221 0.00002 -0.00000 0.00006 0.00005 2.56226

R19 2.03825 -0.00000 0.00001 -0.00001 -0.00000 2.03825

R20 2.03825 -0.00000 0.00001 -0.00001 -0.00000 2.03825

R21 2.66627 -0.00003 -0.00000 -0.00011 -0.00011 2.66615

R22 2.79774 0.00001 0.00006 0.00011 0.00017 2.79791

R23 2.74991 -0.00002 0.00002 -0.00003 -0.00002 2.74990

R24 2.58151 -0.00007 0.00001 -0.00016 -0.00015 2.58136

R25 2.56221 0.00002 -0.00000 0.00006 0.00005 2.56226

R26 2.03825 -0.00000 0.00001 -0.00001 -0.00000 2.03825

R27 2.74991 -0.00002 0.00002 -0.00003 -0.00002 2.74990

R28 2.03825 -0.00000 0.00001 -0.00001 -0.00000 2.03825

R29 2.58151 -0.00007 0.00001 -0.00016 -0.00015 2.58136

R30 2.66627 -0.00003 -0.00000 -0.00011 -0.00011 2.66615

R31 2.67158 0.00004 -0.00010 0.00002 -0.00009 2.67150

R32 2.79774 0.00001 0.00006 0.00011 0.00017 2.79791

R33 2.69503 0.00000 0.00005 0.00005 0.00010 2.69513

R34 2.59012 -0.00004 0.00002 -0.00005 -0.00002 2.59010

R35 2.59666 -0.00004 -0.00007 -0.00008 -0.00015 2.59651

R36 2.03625 -0.00001 0.00001 -0.00003 -0.00002 2.03623

R37 2.69503 0.00000 0.00005 0.00005 0.00010 2.69513

R38 2.03625 -0.00001 0.00001 -0.00003 -0.00002 2.03623

R39 2.59012 -0.00004 0.00002 -0.00005 -0.00002 2.59010

R40 2.67158 0.00004 -0.00010 0.00002 -0.00009 2.67150

R41 1.90975 0.00014 -0.00004 0.00035 0.00031 1.91007

R42 2.79774 0.00001 0.00006 0.00011 0.00017 2.79791

R43 2.65133 -0.00002 -0.00005 -0.00002 -0.00007 2.65126

R44 2.65131 -0.00004 -0.00004 -0.00006 -0.00010 2.65120

R45 2.62810 0.00000 0.00001 0.00003 0.00004 2.62814

R46 2.04814 -0.00000 0.00001 -0.00002 -0.00000 2.04814

R47 2.63518 -0.00001 0.00000 -0.00002 -0.00002 2.63516

R48 2.04946 0.00000 -0.00000 0.00001 0.00001 2.04947

R49 2.63564 -0.00001 0.00000 -0.00003 -0.00002 2.63562

R50 2.04976 -0.00000 0.00000 -0.00000 -0.00000 2.04976

R51 2.62755 0.00001 0.00001 0.00004 0.00005 2.62759

R52 2.04947 -0.00000 -0.00000 0.00001 0.00001 2.04948

R53 2.04789 0.00000 0.00001 -0.00000 0.00001 2.04790

R54 2.63518 -0.00001 0.00000 -0.00002 -0.00002 2.63516

R55 2.63564 -0.00001 0.00000 -0.00003 -0.00002 2.63562

R56 2.04976 -0.00000 0.00000 -0.00000 -0.00000 2.04976

R57 2.62810 0.00000 0.00001 0.00003 0.00004 2.62814

R58 2.04946 0.00000 -0.00000 0.00001 0.00001 2.04947

R59 2.65133 -0.00002 -0.00005 -0.00002 -0.00007 2.65126

R60 2.04814 -0.00000 0.00001 -0.00002 -0.00000 2.04814

R61 2.65131 -0.00004 -0.00004 -0.00006 -0.00010 2.65120

R62 2.62755 0.00001 0.00001 0.00004 0.00005 2.62759

R63 2.04789 0.00000 0.00001 -0.00000 0.00001 2.04790

R64 2.04947 -0.00000 -0.00000 0.00001 0.00001 2.04948

R65 2.65131 -0.00004 -0.00004 -0.00006 -0.00010 2.65120

R66 2.65133 -0.00002 -0.00005 -0.00002 -0.00007 2.65126

R67 2.62755 0.00001 0.00001 0.00004 0.00005 2.62759

R68 2.04789 0.00000 0.00001 -0.00000 0.00001 2.04790

R69 2.63564 -0.00001 0.00000 -0.00003 -0.00002 2.63562

R70 2.04947 -0.00000 -0.00000 0.00001 0.00001 2.04948

R71 2.63518 -0.00001 0.00000 -0.00002 -0.00002 2.63516

R72 2.04976 -0.00000 0.00000 -0.00000 -0.00000 2.04976

R73 2.62810 0.00000 0.00001 0.00003 0.00004 2.62814

R74 2.04946 0.00000 -0.00000 0.00001 0.00001 2.04947

R75 2.04814 -0.00000 0.00001 -0.00002 -0.00000 2.04814

R76 2.65131 -0.00004 -0.00004 -0.00006 -0.00010 2.65120

R77 2.65133 -0.00002 -0.00005 -0.00002 -0.00007 2.65126

R78 2.62755 0.00001 0.00001 0.00004 0.00005 2.62759

R79 2.04789 0.00000 0.00001 -0.00000 0.00001 2.04790

R80 2.63564 -0.00001 0.00000 -0.00003 -0.00002 2.63562

R81 2.04947 -0.00000 -0.00000 0.00001 0.00001 2.04948

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R83 2.04976 -0.00000 0.00000 -0.00000 -0.00000 2.04976

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R85 2.04946 0.00000 -0.00000 0.00001 0.00001 2.04947

R86 2.04814 -0.00000 0.00001 -0.00002 -0.00000 2.04814

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A2 2.18317 -0.00002 -0.00005 -0.00016 -0.00020 2.18297

A3 2.21666 0.00003 0.00002 0.00019 0.00020 2.21686

A4 1.86602 0.00003 -0.00006 0.00013 0.00007 1.86608

A5 2.21509 -0.00002 0.00003 -0.00011 -0.00008 2.21501

A6 2.20193 -0.00000 0.00004 -0.00004 0.00000 2.20193

A7 1.92591 -0.00002 0.00006 -0.00012 -0.00006 1.92585

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A9 2.17863 0.00001 -0.00003 0.00005 0.00002 2.17865

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A15 2.18317 -0.00002 -0.00005 -0.00016 -0.00020 2.18297

A16 2.18099 0.00003 0.00011 -0.00002 0.00010 2.18109

A17 2.03723 0.00004 -0.00003 0.00021 0.00017 2.03740

A18 2.06495 -0.00007 -0.00008 -0.00019 -0.00027 2.06468

A19 2.18360 -0.00004 0.00012 -0.00018 -0.00006 2.18354

A20 2.16494 0.00002 -0.00008 0.00009 0.00001 2.16494

A21 1.93440 0.00003 -0.00003 0.00009 0.00006 1.93446

A22 1.84225 -0.00000 0.00003 -0.00010 -0.00007 1.84219

A23 1.93440 0.00003 -0.00003 0.00009 0.00006 1.93446

A24 2.18360 -0.00004 0.00012 -0.00018 -0.00006 2.18354

A25 2.16494 0.00002 -0.00008 0.00009 0.00001 2.16494

A26 1.85631 -0.00003 0.00001 -0.00009 -0.00007 1.85624

A27 2.19999 -0.00001 -0.00003 -0.00006 -0.00009 2.19990

A28 2.22644 0.00003 0.00002 0.00016 0.00018 2.22662

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A32 2.18099 0.00003 0.00011 -0.00002 0.00010 2.18109

A33 2.03723 0.00004 -0.00003 0.00021 0.00017 2.03740

A34 2.06495 -0.00007 -0.00008 -0.00019 -0.00027 2.06468

A35 2.16494 0.00002 -0.00008 0.00009 0.00001 2.16494

A36 2.18360 -0.00004 0.00012 -0.00018 -0.00006 2.18354

A37 1.93440 0.00003 -0.00003 0.00009 0.00006 1.93446

A38 1.85631 -0.00003 0.00001 -0.00009 -0.00007 1.85624

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A43 2.19999 -0.00001 -0.00003 -0.00006 -0.00009 2.19990

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A46 2.18360 -0.00004 0.00012 -0.00018 -0.00006 2.18354

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A54 1.88302 -0.00001 0.00003 -0.00004 -0.00001 1.88302

A55 2.18317 -0.00002 -0.00005 -0.00016 -0.00020 2.18297

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A70 2.09951 -0.00007 -0.00001 -0.00025 -0.00025 2.09926

A71 2.07879 0.00007 0.00002 0.00019 0.00021 2.07900

A72 2.10030 -0.00004 -0.00000 -0.00013 -0.00013 2.10018

A73 2.08716 0.00002 0.00000 0.00007 0.00007 2.08723

A74 2.09536 0.00001 0.00000 0.00005 0.00005 2.09541

A75 2.09710 -0.00000 -0.00000 -0.00001 -0.00001 2.09709

A76 2.08873 0.00000 -0.00001 0.00002 0.00001 2.08874

A77 2.09735 0.00000 0.00001 -0.00001 -0.00000 2.09735

A78 2.09241 0.00002 -0.00001 0.00006 0.00005 2.09246

A79 2.09541 -0.00001 0.00001 -0.00003 -0.00003 2.09538

A80 2.09536 -0.00001 0.00001 -0.00003 -0.00002 2.09534

A81 2.09712 -0.00000 -0.00000 -0.00001 -0.00001 2.09711

A82 2.09728 0.00000 0.00001 -0.00001 0.00000 2.09728

A83 2.08879 -0.00000 -0.00001 0.00001 0.00000 2.08879

A84 2.10043 -0.00004 -0.00000 -0.00012 -0.00012 2.10031

A85 2.08631 0.00001 0.00000 0.00001 0.00001 2.08632

A86 2.09610 0.00003 0.00000 0.00011 0.00011 2.09621

A87 2.09241 0.00002 -0.00001 0.00006 0.00005 2.09246

A88 2.09541 -0.00001 0.00001 -0.00003 -0.00003 2.09538

A89 2.09536 -0.00001 0.00001 -0.00003 -0.00002 2.09534

A90 2.09710 -0.00000 -0.00000 -0.00001 -0.00001 2.09709

A91 2.09735 0.00000 0.00001 -0.00001 -0.00000 2.09735

A92 2.08873 0.00000 -0.00001 0.00002 0.00001 2.08874

A93 2.10030 -0.00004 -0.00000 -0.00013 -0.00013 2.10018

A94 2.09536 0.00001 0.00000 0.00005 0.00005 2.09541

A95 2.08716 0.00002 0.00000 0.00007 0.00007 2.08723

A96 2.10489 0.00001 -0.00001 0.00006 0.00005 2.10493

A97 2.09951 -0.00007 -0.00001 -0.00025 -0.00025 2.09926

A98 2.07879 0.00007 0.00002 0.00019 0.00021 2.07900

A99 2.10043 -0.00004 -0.00000 -0.00012 -0.00012 2.10031

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A103 2.09728 0.00000 0.00001 -0.00001 0.00000 2.09728

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A107 2.07879 0.00007 0.00002 0.00019 0.00021 2.07900

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A109 2.08631 0.00001 0.00000 0.00001 0.00001 2.08632

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A111 2.09712 -0.00000 -0.00000 -0.00001 -0.00001 2.09711

A112 2.08879 -0.00000 -0.00001 0.00001 0.00000 2.08879

A113 2.09728 0.00000 0.00001 -0.00001 0.00000 2.09728

A114 2.09241 0.00002 -0.00001 0.00006 0.00005 2.09246

A115 2.09536 -0.00001 0.00001 -0.00003 -0.00002 2.09534

A116 2.09541 -0.00001 0.00001 -0.00003 -0.00003 2.09538

A117 2.09710 -0.00000 -0.00000 -0.00001 -0.00001 2.09709

A118 2.09735 0.00000 0.00001 -0.00001 -0.00000 2.09735

A119 2.08873 0.00000 -0.00001 0.00002 0.00001 2.08874

A120 2.10030 -0.00004 -0.00000 -0.00013 -0.00013 2.10018

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A122 2.09536 0.00001 0.00000 0.00005 0.00005 2.09541

A123 2.09951 -0.00007 -0.00001 -0.00025 -0.00025 2.09926

A124 2.10489 0.00001 -0.00001 0.00006 0.00005 2.10493

A125 2.07879 0.00007 0.00002 0.00019 0.00021 2.07900

A126 2.10043 -0.00004 -0.00000 -0.00012 -0.00012 2.10031

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A128 2.09610 0.00003 0.00000 0.00011 0.00011 2.09621

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A133 2.09536 -0.00001 0.00001 -0.00003 -0.00002 2.09534

A134 2.09541 -0.00001 0.00001 -0.00003 -0.00003 2.09538

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A137 2.08873 0.00000 -0.00001 0.00002 0.00001 2.08874

A138 2.10030 -0.00004 -0.00000 -0.00013 -0.00013 2.10018

A139 2.08716 0.00002 0.00000 0.00007 0.00007 2.08723

A140 2.09536 0.00001 0.00000 0.00005 0.00005 2.09541

D1 0.02223 -0.00001 0.00003 -0.00078 -0.00075 0.02147

D2 -3.10164 0.00000 -0.00023 0.00030 0.00007 -3.10157

D3 -3.09333 -0.00001 -0.00011 -0.00041 -0.00052 -3.09385

D4 0.06599 0.00001 -0.00037 0.00067 0.00030 0.06629

D5 0.00000 0.00000 0.00000 0.00000 -0.00000 0.00000

D6 -3.11492 0.00001 -0.00014 0.00038 0.00025 -3.11467

D7 3.11492 -0.00001 0.00014 -0.00038 -0.00025 3.11467

D8 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D9 -0.03704 0.00002 -0.00005 0.00130 0.00125 -0.03579

D10 3.09735 -0.00002 -0.00007 -0.00087 -0.00094 3.09641

D11 3.08700 0.00000 0.00021 0.00024 0.00044 3.08744

D12 -0.06180 -0.00004 0.00019 -0.00194 -0.00175 -0.06355

D13 -2.97374 -0.00003 -0.00048 -0.00165 -0.00213 -2.97587

D14 0.16306 -0.00003 -0.00054 -0.00163 -0.00217 0.16089

D15 0.18886 -0.00002 -0.00079 -0.00038 -0.00116 0.18769

D16 -2.95753 -0.00002 -0.00084 -0.00036 -0.00120 -2.95873

D17 0.03704 -0.00002 0.00005 -0.00130 -0.00125 0.03579

D18 -3.08700 -0.00000 -0.00021 -0.00024 -0.00044 -3.08744

D19 -3.09735 0.00002 0.00007 0.00087 0.00094 -3.09641

D20 0.06180 0.00004 -0.00019 0.00194 0.00175 0.06355

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D22 3.09333 0.00001 0.00011 0.00041 0.00052 3.09385

D23 3.10164 -0.00000 0.00023 -0.00030 -0.00007 3.10157

D24 -0.06599 -0.00001 0.00037 -0.00067 -0.00030 -0.06629

D25 -0.18886 0.00002 0.00079 0.00038 0.00116 -0.18769

D26 2.95753 0.00002 0.00084 0.00036 0.00120 2.95873

D27 2.97374 0.00003 0.00048 0.00165 0.00213 2.97587

D28 -0.16306 0.00003 0.00054 0.00163 0.00217 -0.16089

D29 -0.18314 0.00001 0.00088 -0.00022 0.00067 -0.18247

D30 2.98449 -0.00000 0.00060 -0.00042 0.00017 2.98466

D31 2.95359 0.00001 0.00083 -0.00019 0.00063 2.95422

D32 -0.16197 -0.00000 0.00054 -0.00040 0.00014 -0.16183

D33 -0.96737 -0.00001 -0.00024 -0.00097 -0.00122 -0.96858

D34 2.17332 -0.00000 -0.00019 -0.00077 -0.00096 2.17236

D35 2.17869 -0.00001 -0.00019 -0.00100 -0.00118 2.17750

D36 -0.96381 -0.00000 -0.00014 -0.00079 -0.00093 -0.96473

D37 -3.07526 0.00004 -0.00007 0.00136 0.00129 -3.07397

D38 0.04325 0.00005 0.00018 0.00154 0.00173 0.04497

D39 3.09154 -0.00002 0.00014 -0.00080 -0.00066 3.09088

D40 -0.08036 -0.00000 0.00035 -0.00051 -0.00016 -0.08051

D41 -0.02726 -0.00003 -0.00012 -0.00097 -0.00109 -0.02835

D42 3.08403 -0.00001 0.00010 -0.00069 -0.00059 3.08344

D43 -0.04325 -0.00005 -0.00018 -0.00154 -0.00173 -0.04497

D44 3.07526 -0.00004 0.00007 -0.00136 -0.00129 3.07397

D45 0.02726 0.00003 0.00012 0.00097 0.00109 0.02835

D46 -3.08403 0.00001 -0.00010 0.00069 0.00059 -3.08344

D47 -3.09154 0.00002 -0.00014 0.00080 0.00066 -3.09088

D48 0.08036 0.00000 -0.00035 0.00051 0.00016 0.08051

D49 0.18314 -0.00001 -0.00088 0.00022 -0.00067 0.18247

D50 -2.95359 -0.00001 -0.00083 0.00019 -0.00063 -2.95422

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D52 0.16197 0.00000 -0.00054 0.00040 -0.00014 0.16183

D53 -0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D54 -3.11068 -0.00002 -0.00022 -0.00029 -0.00050 -3.11119

D55 3.11068 0.00002 0.00022 0.00029 0.00050 3.11119

D56 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D57 -2.98449 0.00000 -0.00060 0.00042 -0.00017 -2.98466

D58 0.18314 -0.00001 -0.00088 0.00022 -0.00067 0.18247

D59 0.16197 0.00000 -0.00054 0.00040 -0.00014 0.16183

D60 -2.95359 -0.00001 -0.00083 0.00019 -0.00063 -2.95422

D61 0.96737 0.00001 0.00024 0.00097 0.00122 0.96858

D62 -2.17332 0.00000 0.00019 0.00077 0.00096 -2.17236

D63 -2.17869 0.00001 0.00019 0.00100 0.00118 -2.17750

D64 0.96381 0.00000 0.00014 0.00079 0.00093 0.96473

D65 -3.09154 0.00002 -0.00014 0.00080 0.00066 -3.09088

D66 0.08036 0.00000 -0.00035 0.00051 0.00016 0.08051

D67 0.02726 0.00003 0.00012 0.00097 0.00109 0.02835

D68 -3.08403 0.00001 -0.00010 0.00069 0.00059 -3.08344

D69 3.07526 -0.00004 0.00007 -0.00136 -0.00129 3.07397

D70 -0.04325 -0.00005 -0.00018 -0.00154 -0.00173 -0.04497

D71 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D72 -3.11068 -0.00002 -0.00022 -0.00029 -0.00050 -3.11119

D73 3.11068 0.00002 0.00022 0.00029 0.00050 3.11119

D74 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D75 -0.02726 -0.00003 -0.00012 -0.00097 -0.00109 -0.02835

D76 3.09154 -0.00002 0.00014 -0.00080 -0.00066 3.09088

D77 3.08403 -0.00001 0.00010 -0.00069 -0.00059 3.08344

D78 -0.08036 -0.00000 0.00035 -0.00051 -0.00016 -0.08051

D79 0.04325 0.00005 0.00018 0.00154 0.00173 0.04497

D80 -3.07526 0.00004 -0.00007 0.00136 0.00129 -3.07397

D81 2.98449 -0.00000 0.00060 -0.00042 0.00017 2.98466

D82 -0.16197 -0.00000 0.00054 -0.00040 0.00014 -0.16183

D83 -0.18314 0.00001 0.00088 -0.00022 0.00067 -0.18247

D84 2.95359 0.00001 0.00083 -0.00019 0.00063 2.95422

D85 2.97374 0.00003 0.00048 0.00165 0.00213 2.97587

D86 -0.18886 0.00002 0.00079 0.00038 0.00116 -0.18769

D87 -0.16306 0.00003 0.00054 0.00163 0.00217 -0.16089

D88 2.95753 0.00002 0.00084 0.00036 0.00120 2.95873

D89 -0.96381 -0.00000 -0.00014 -0.00079 -0.00093 -0.96473

D90 2.17869 -0.00001 -0.00019 -0.00100 -0.00118 2.17750

D91 2.17332 -0.00000 -0.00019 -0.00077 -0.00096 2.17236

D92 -0.96737 -0.00001 -0.00024 -0.00097 -0.00122 -0.96858

D93 3.10164 -0.00000 0.00023 -0.00030 -0.00007 3.10157

D94 -0.06599 -0.00001 0.00037 -0.00067 -0.00030 -0.06629

D95 -0.02223 0.00001 -0.00003 0.00078 0.00075 -0.02147

D96 3.09333 0.00001 0.00011 0.00041 0.00052 3.09385

D97 -3.08700 -0.00000 -0.00021 -0.00024 -0.00044 -3.08744

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D99 0.03704 -0.00002 0.00005 -0.00130 -0.00125 0.03579

D100 -3.09735 0.00002 0.00007 0.00087 0.00094 -3.09641

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D103 -3.11492 0.00001 -0.00014 0.00038 0.00025 -3.11467

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D106 -3.10164 0.00000 -0.00023 0.00030 0.00007 -3.10157

D107 -3.09333 -0.00001 -0.00011 -0.00041 -0.00052 -3.09385

D108 0.06599 0.00001 -0.00037 0.00067 0.00030 0.06629

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D114 0.16306 -0.00003 -0.00054 -0.00163 -0.00217 0.16089

D115 0.18886 -0.00002 -0.00079 -0.00038 -0.00116 0.18769

D116 -2.95753 -0.00002 -0.00084 -0.00036 -0.00120 -2.95873

D117 0.96381 0.00000 0.00014 0.00079 0.00093 0.96473

D118 -2.17869 0.00001 0.00019 0.00100 0.00118 -2.17750

D119 -2.17332 0.00000 0.00019 0.00077 0.00096 -2.17236

D120 0.96737 0.00001 0.00024 0.00097 0.00122 0.96858

D121 -3.13244 0.00000 -0.00000 -0.00000 -0.00001 -3.13245

D122 -0.01978 -0.00000 0.00013 -0.00013 0.00000 -0.01977

D123 0.01004 -0.00000 -0.00006 -0.00021 -0.00026 0.00978

D124 3.12271 -0.00001 0.00008 -0.00033 -0.00025 3.12246

D125 -3.13236 0.00000 -0.00004 0.00011 0.00007 -3.13229

D126 -0.01877 0.00000 0.00009 -0.00003 0.00006 -0.01871

D127 0.00834 0.00001 0.00001 0.00031 0.00033 0.00867

D128 3.12193 0.00001 0.00014 0.00017 0.00031 3.12224

D129 -0.01874 -0.00000 0.00006 -0.00003 0.00002 -0.01872

D130 3.12291 -0.00000 0.00009 -0.00013 -0.00004 3.12287

D131 -3.13127 0.00000 -0.00008 0.00009 0.00001 -3.13126

D132 0.01038 -0.00000 -0.00005 -0.00000 -0.00005 0.01033

D133 0.00901 0.00000 -0.00001 0.00017 0.00016 0.00917

D134 -3.13235 0.00000 -0.00003 0.00004 0.00001 -3.13233

D135 -3.13264 0.00001 -0.00005 0.00027 0.00022 -3.13242

D136 0.00919 0.00000 -0.00006 0.00014 0.00008 0.00927

D137 0.00938 -0.00000 -0.00003 -0.00007 -0.00009 0.00928

D138 -3.13212 -0.00000 -0.00007 -0.00003 -0.00010 -3.13222

D139 -3.13245 0.00000 -0.00002 0.00007 0.00005 -3.13240

D140 0.00924 0.00000 -0.00006 0.00010 0.00004 0.00928

D141 -0.01807 -0.00000 0.00003 -0.00018 -0.00015 -0.01821

D142 -3.13150 -0.00000 -0.00010 -0.00003 -0.00013 -3.13163

D143 3.12343 -0.00000 0.00007 -0.00021 -0.00014 3.12329

D144 0.01000 -0.00000 -0.00006 -0.00007 -0.00012 0.00987

D145 -0.00901 -0.00000 0.00001 -0.00017 -0.00016 -0.00917

D146 3.13264 -0.00001 0.00005 -0.00027 -0.00022 3.13242

D147 3.13235 -0.00000 0.00003 -0.00004 -0.00001 3.13233

D148 -0.00919 -0.00000 0.00006 -0.00014 -0.00008 -0.00927

D149 -0.00938 0.00000 0.00003 0.00007 0.00009 -0.00928

D150 3.13212 0.00000 0.00007 0.00003 0.00010 3.13222

D151 3.13245 -0.00000 0.00002 -0.00007 -0.00005 3.13240

D152 -0.00924 -0.00000 0.00006 -0.00010 -0.00004 -0.00928

D153 0.01874 0.00000 -0.00006 0.00003 -0.00002 0.01872

D154 3.13127 -0.00000 0.00008 -0.00009 -0.00001 3.13126

D155 -3.12291 0.00000 -0.00009 0.00013 0.00004 -3.12287

D156 -0.01038 0.00000 0.00005 0.00000 0.00005 -0.01033

D157 3.13244 -0.00000 0.00000 0.00000 0.00001 3.13245

D158 -0.01004 0.00000 0.00006 0.00021 0.00026 -0.00978

D159 0.01978 0.00000 -0.00013 0.00013 -0.00000 0.01977

D160 -3.12271 0.00001 -0.00008 0.00033 0.00025 -3.12246

D161 3.13236 -0.00000 0.00004 -0.00011 -0.00007 3.13229

D162 0.01877 -0.00000 -0.00009 0.00003 -0.00006 0.01871

D163 -0.00834 -0.00001 -0.00001 -0.00031 -0.00033 -0.00867

D164 -3.12193 -0.00001 -0.00014 -0.00017 -0.00031 -3.12224

D165 0.01807 0.00000 -0.00003 0.00018 0.00015 0.01821

D166 -3.12343 0.00000 -0.00007 0.00021 0.00014 -3.12329

D167 3.13150 0.00000 0.00010 0.00003 0.00013 3.13163

D168 -0.01000 0.00000 0.00006 0.00007 0.00012 -0.00987

D169 3.13236 -0.00000 0.00004 -0.00011 -0.00007 3.13229

D170 0.01877 -0.00000 -0.00009 0.00003 -0.00006 0.01871

D171 -0.00834 -0.00001 -0.00001 -0.00031 -0.00033 -0.00867

D172 -3.12193 -0.00001 -0.00014 -0.00017 -0.00031 -3.12224

D173 3.13244 -0.00000 0.00000 0.00000 0.00001 3.13245

D174 0.01978 0.00000 -0.00013 0.00013 -0.00000 0.01977

D175 -0.01004 0.00000 0.00006 0.00021 0.00026 -0.00978

D176 -3.12271 0.00001 -0.00008 0.00033 0.00025 -3.12246

D177 0.01807 0.00000 -0.00003 0.00018 0.00015 0.01821

D178 -3.12343 0.00000 -0.00007 0.00021 0.00014 -3.12329

D179 3.13150 0.00000 0.00010 0.00003 0.00013 3.13163

D180 -0.01000 0.00000 0.00006 0.00007 0.00012 -0.00987

D181 -0.00938 0.00000 0.00003 0.00007 0.00009 -0.00928

D182 3.13245 -0.00000 0.00002 -0.00007 -0.00005 3.13240

D183 3.13212 0.00000 0.00007 0.00003 0.00010 3.13222

D184 -0.00924 -0.00000 0.00006 -0.00010 -0.00004 -0.00928

D185 -0.00901 -0.00000 0.00001 -0.00017 -0.00016 -0.00917

D186 3.13264 -0.00001 0.00005 -0.00027 -0.00022 3.13242

D187 3.13235 -0.00000 0.00003 -0.00004 -0.00001 3.13233

D188 -0.00919 -0.00000 0.00006 -0.00014 -0.00008 -0.00927

D189 0.01874 0.00000 -0.00006 0.00003 -0.00002 0.01872

D190 3.13127 -0.00000 0.00008 -0.00009 -0.00001 3.13126

D191 -3.12291 0.00000 -0.00009 0.00013 0.00004 -3.12287

D192 -0.01038 0.00000 0.00005 0.00000 0.00005 -0.01033

D193 -3.13236 0.00000 -0.00004 0.00011 0.00007 -3.13229

D194 -0.01877 0.00000 0.00009 -0.00003 0.00006 -0.01871

D195 0.00834 0.00001 0.00001 0.00031 0.00033 0.00867

D196 3.12193 0.00001 0.00014 0.00017 0.00031 3.12224

D197 -3.13244 0.00000 -0.00000 -0.00000 -0.00001 -3.13245

D198 -0.01978 -0.00000 0.00013 -0.00013 0.00000 -0.01977

D199 0.01004 -0.00000 -0.00006 -0.00021 -0.00026 0.00978

D200 3.12271 -0.00001 0.00008 -0.00033 -0.00025 3.12246

D201 -0.01807 -0.00000 0.00003 -0.00018 -0.00015 -0.01821

D202 3.12343 -0.00000 0.00007 -0.00021 -0.00014 3.12329

D203 -3.13150 -0.00000 -0.00010 -0.00003 -0.00013 -3.13163

D204 0.01000 -0.00000 -0.00006 -0.00007 -0.00012 0.00987

D205 0.00938 -0.00000 -0.00003 -0.00007 -0.00009 0.00928

D206 -3.13245 0.00000 -0.00002 0.00007 0.00005 -3.13240

D207 -3.13212 -0.00000 -0.00007 -0.00003 -0.00010 -3.13222

D208 0.00924 0.00000 -0.00006 0.00010 0.00004 0.00928

D209 0.00901 0.00000 -0.00001 0.00017 0.00016 0.00917

D210 -3.13264 0.00001 -0.00005 0.00027 0.00022 -3.13242

D211 -3.13235 0.00000 -0.00003 0.00004 0.00001 -3.13233

D212 0.00919 0.00000 -0.00006 0.00014 0.00008 0.00927

D213 -0.01874 -0.00000 0.00006 -0.00003 0.00002 -0.01872

D214 -3.13127 0.00000 -0.00008 0.00009 0.00001 -3.13126

D215 3.12291 -0.00000 0.00009 -0.00013 -0.00004 3.12287

D216 0.01038 -0.00000 -0.00005 -0.00000 -0.00005 0.01033

Item Value Threshold Converged?

Maximum Force 0.000138 0.000450 YES

RMS Force 0.000024 0.000300 YES

Maximum Displacement 0.008794 0.001800 NO

RMS Displacement 0.002382 0.001200 NO

Predicted change in Energy=-1.458408D-06

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Aug 18 14:32:06 2019, MaxMem= 2013265920 cpu: 1.4

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

Stoichiometry C44H30N4(1+,2)

Framework group C2V[SGV(H2N2),SGV'(N2),X(C44H28)]

Deg. of freedom 59

Full point group C2V NOp 4

RotChk: IX=0 Diff= 3.36D-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 -0.687007 4.173124 0.509577

2 6 0 -1.125094 2.863441 0.153411

3 7 0 0.000000 2.101184 -0.024704

4 6 0 1.125094 2.863441 0.153411

5 6 0 0.687007 4.173124 0.509577

6 6 0 2.460733 2.430424 -0.011212

7 6 0 2.860787 1.087693 -0.177283

8 7 0 2.053003 -0.000000 -0.003053

9 6 0 2.860787 -1.087693 -0.177283

10 6 0 4.211501 -0.677944 -0.531168

11 6 0 4.211501 0.677944 -0.531168

12 6 0 -2.460733 2.430424 -0.011212

13 6 0 -2.860787 1.087693 -0.177283

14 6 0 -4.211501 0.677944 -0.531168

15 6 0 -4.211501 -0.677944 -0.531168

16 6 0 -2.860787 -1.087693 -0.177283

17 7 0 -2.053003 0.000000 -0.003053

18 6 0 -2.460733 -2.430424 -0.011212

19 6 0 -1.125094 -2.863441 0.153411

20 6 0 -0.687007 -4.173124 0.509577

21 6 0 0.687007 -4.173124 0.509577

22 6 0 1.125094 -2.863441 0.153411

23 7 0 -0.000000 -2.101184 -0.024704

24 6 0 2.460733 -2.430424 -0.011212

25 6 0 3.506761 3.478205 -0.000196

26 6 0 3.441893 4.561610 -0.889240

27 6 0 4.433308 5.536916 -0.881386

28 6 0 5.488320 5.456032 0.026876

29 6 0 5.554615 4.388413 0.921868

30 6 0 4.577485 3.399350 0.902921

31 6 0 -5.488320 5.456032 0.026876

32 6 0 -4.433308 5.536916 -0.881386

33 6 0 -3.441893 4.561610 -0.889240

34 6 0 -3.506761 3.478205 -0.000196

35 6 0 -4.577485 3.399350 0.902921

36 6 0 -5.554615 4.388413 0.921868

37 6 0 3.506761 -3.478205 -0.000196

38 6 0 4.577485 -3.399350 0.902921

39 6 0 5.554615 -4.388413 0.921868

40 6 0 5.488320 -5.456032 0.026876

41 6 0 4.433308 -5.536916 -0.881386

42 6 0 3.441893 -4.561610 -0.889240

43 6 0 -3.506761 -3.478205 -0.000196

44 6 0 -4.577485 -3.399350 0.902921

45 6 0 -5.554615 -4.388413 0.921868

46 6 0 -5.488320 -5.456032 0.026876

47 6 0 -4.433308 -5.536916 -0.881386

48 6 0 -3.441893 -4.561610 -0.889240

49 1 0 -1.335729 4.996953 0.757617

50 1 0 1.335729 4.996953 0.757617

51 1 0 5.031459 -1.335683 -0.772861

52 1 0 5.031459 1.335683 -0.772861

53 1 0 -5.031459 1.335683 -0.772861

54 1 0 -5.031459 -1.335683 -0.772861

55 1 0 -1.335729 -4.996953 0.757617

56 1 0 1.335729 -4.996953 0.757617

57 1 0 2.627747 4.620831 -1.602223

58 1 0 4.381838 6.360568 -1.585059

59 1 0 6.256085 6.222173 0.037376

60 1 0 6.368438 4.325660 1.635993

61 1 0 4.624752 2.575057 1.604857

62 1 0 -6.256085 6.222173 0.037376

63 1 0 -4.381838 6.360568 -1.585059

64 1 0 -2.627747 4.620831 -1.602223

65 1 0 -4.624752 2.575057 1.604857

66 1 0 -6.368438 4.325660 1.635993

67 1 0 4.624752 -2.575057 1.604857

68 1 0 6.368438 -4.325660 1.635993

69 1 0 6.256085 -6.222173 0.037376

70 1 0 4.381838 -6.360568 -1.585059

71 1 0 2.627747 -4.620831 -1.602223

72 1 0 -4.624752 -2.575057 1.604857

73 1 0 -6.368438 -4.325660 1.635993

74 1 0 -6.256085 -6.222173 0.037376

75 1 0 -4.381838 -6.360568 -1.585059

76 1 0 -2.627747 -4.620831 -1.602223

77 1 0 0.000000 1.115189 -0.247093

78 1 0 -0.000000 -1.115189 -0.247093

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

Rotational constants (GHZ): 0.0592984 0.0586044 0.0302886

Leave Link 202 at Sun Aug 18 14:32:07 2019, MaxMem= 2013265920 cpu: 0.1

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

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

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

There are 261 symmetry adapted cartesian basis functions of A1 symmetry.

There are 240 symmetry adapted cartesian basis functions of A2 symmetry.

There are 249 symmetry adapted cartesian basis functions of B1 symmetry.

There are 252 symmetry adapted cartesian basis functions of B2 symmetry.

There are 248 symmetry adapted basis functions of A1 symmetry.

There are 229 symmetry adapted basis functions of A2 symmetry.

There are 237 symmetry adapted basis functions of B1 symmetry.

There are 240 symmetry adapted basis functions of B2 symmetry.

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

161 alpha electrons 160 beta electrons

nuclear repulsion energy 5372.1326753273 Hartrees.

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

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

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

NAtoms= 78 NActive= 78 NUniq= 21 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=T Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2128235466 Hartrees.

Nuclear repulsion after empirical dispersion term = 5371.9198517807 Hartrees.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 78

GePol: Total number of spheres = 78

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

GePol: Number of points = 5706

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.27D-10

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 294

GePol: Fraction of low-weight points (<1% of avg) = 5.15%

GePol: Cavity surface area = 608.651 Ang\*\*2

GePol: Cavity volume = 626.254 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0022213033 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5371.9176304774 Hartrees.

Leave Link 301 at Sun Aug 18 14:32:07 2019, MaxMem= 2013265920 cpu: 1.0

(Enter /home/kira/g09/l302.exe)

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

NBasis= 954 RedAO= T EigKep= 6.37D-05 NBF= 248 229 237 240

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 248 229 237 240

Precomputing XC quadrature grid using

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

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

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

Leave Link 302 at Sun Aug 18 14:32:08 2019, MaxMem= 2013265920 cpu: 9.5

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

DipDrv: MaxL=1.

Leave Link 303 at Sun Aug 18 14:32:08 2019, MaxMem= 2013265920 cpu: 1.3

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

Initial guess from the checkpoint file: "TPPcation.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) (B1) (A1) (B2) (A2) (A1) (B1) (A2) (B2)

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

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The electronic state of the initial guess is 2-A1.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7873 S= 0.5185

Leave Link 401 at Sun Aug 18 14:32:12 2019, MaxMem= 2013265920 cpu: 33.3

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3049894 IEndB= 3049894 NGot= 2013265920 MDV= 2011237673

LenX= 2011237673 LenY= 2010232667

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

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

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

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

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

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 97675308.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.44D-15 for 5690.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.66D-15 for 5684 4639.

Iteration 1 A^-1\*A deviation from unit magnitude is 8.66D-15 for 5690.

Iteration 1 A^-1\*A deviation from orthogonality is 1.40D-12 for 1888 1885.

E= -1914.20121330346

DIIS: error= 1.37D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.20121330346 IErMin= 1 ErrMin= 1.37D-04

ErrMax= 1.37D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.02D-05 BMatP= 6.02D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.37D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.503 Goal= None Shift= 0.000

Gap= 0.515 Goal= None Shift= 0.000

RMSDP=6.07D-06 MaxDP=1.49D-04 OVMax= 9.62D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 6.07D-06 CP: 1.00D+00

E= -1914.20124012600 Delta-E= -0.000026822538 Rises=F Damp=F

DIIS: error= 1.77D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.20124012600 IErMin= 2 ErrMin= 1.77D-05

ErrMax= 1.77D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.48D-07 BMatP= 6.02D-05

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

Coeff-Com: -0.587D-01 0.106D+01

Coeff: -0.587D-01 0.106D+01

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=1.18D-06 MaxDP=5.22D-05 DE=-2.68D-05 OVMax= 2.42D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.11D-06 CP: 1.00D+00 1.06D+00

E= -1914.20124035984 Delta-E= -0.000000233848 Rises=F Damp=F

DIIS: error= 2.00D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.20124035984 IErMin= 2 ErrMin= 1.77D-05

ErrMax= 2.00D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.43D-07 BMatP= 8.48D-07

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

Coeff-Com: -0.390D-01 0.572D+00 0.467D+00

Coeff: -0.390D-01 0.572D+00 0.467D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=6.72D-07 MaxDP=4.93D-05 DE=-2.34D-07 OVMax= 1.95D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 4.31D-07 CP: 1.00D+00 1.07D+00 5.44D-01

E= -1914.20124052998 Delta-E= -0.000000170138 Rises=F Damp=F

DIIS: error= 8.12D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.20124052998 IErMin= 4 ErrMin= 8.12D-06

ErrMax= 8.12D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.21D-07 BMatP= 8.43D-07

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

Coeff-Com: -0.105D-01 0.125D+00 0.280D+00 0.606D+00

Coeff: -0.105D-01 0.125D+00 0.280D+00 0.606D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=2.40D-07 MaxDP=1.97D-05 DE=-1.70D-07 OVMax= 9.58D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.37D-07 CP: 1.00D+00 1.08D+00 6.75D-01 7.01D-01

E= -1914.20124055682 Delta-E= -0.000000026837 Rises=F Damp=F

DIIS: error= 1.88D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.20124055682 IErMin= 5 ErrMin= 1.88D-06

ErrMax= 1.88D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.05D-08 BMatP= 1.21D-07

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

Coeff-Com: -0.202D-02 0.124D-01 0.104D+00 0.317D+00 0.568D+00

Coeff: -0.202D-02 0.124D-01 0.104D+00 0.317D+00 0.568D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=6.84D-08 MaxDP=4.64D-06 DE=-2.68D-08 OVMax= 2.19D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 4.79D-08 CP: 1.00D+00 1.08D+00 6.66D-01 7.88D-01 7.93D-01

E= -1914.20124055919 Delta-E= -0.000000002367 Rises=F Damp=F

DIIS: error= 7.38D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.20124055919 IErMin= 6 ErrMin= 7.38D-07

ErrMax= 7.38D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.56D-09 BMatP= 1.05D-08

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

Coeff-Com: 0.101D-02-0.199D-01 0.786D-03 0.553D-01 0.305D+00 0.658D+00

Coeff: 0.101D-02-0.199D-01 0.786D-03 0.553D-01 0.305D+00 0.658D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=3.02D-08 MaxDP=1.93D-06 DE=-2.37D-09 OVMax= 1.51D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.03D-08 CP: 1.00D+00 1.08D+00 6.81D-01 7.96D-01 8.78D-01

CP: 8.26D-01

E= -1914.20124055970 Delta-E= -0.000000000515 Rises=F Damp=F

DIIS: error= 2.73D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.20124055970 IErMin= 7 ErrMin= 2.73D-07

ErrMax= 2.73D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.84D-10 BMatP= 1.56D-09

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

Coeff-Com: 0.644D-03-0.107D-01-0.656D-02 0.674D-02 0.107D+00 0.325D+00

Coeff-Com: 0.578D+00

Coeff: 0.644D-03-0.107D-01-0.656D-02 0.674D-02 0.107D+00 0.325D+00

Coeff: 0.578D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=1.03D-08 MaxDP=4.65D-07 DE=-5.15D-10 OVMax= 5.24D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 8.76D-09 CP: 1.00D+00 1.08D+00 6.82D-01 8.02D-01 8.93D-01

CP: 9.10D-01 1.04D+00

E= -1914.20124055977 Delta-E= -0.000000000072 Rises=F Damp=F

DIIS: error= 1.48D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.20124055977 IErMin= 8 ErrMin= 1.48D-07

ErrMax= 1.48D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.99D-11 BMatP= 1.84D-10

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

Coeff-Com: -0.141D-03 0.365D-02-0.272D-02-0.173D-01-0.820D-01-0.136D+00

Coeff-Com: 0.256D+00 0.979D+00

Coeff: -0.141D-03 0.365D-02-0.272D-02-0.173D-01-0.820D-01-0.136D+00

Coeff: 0.256D+00 0.979D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=9.26D-09 MaxDP=6.41D-07 DE=-7.19D-11 OVMax= 6.98D-06

Error on total polarization charges = 0.07902

SCF Done: E(UB3LYP) = -1914.20124056 A.U. after 8 cycles

NFock= 8 Conv=0.93D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7873 S= 0.5185

<L.S>= 0.000000000000E+00

KE= 1.906180710068D+03 PE=-1.515842458045D+04 EE= 5.966124999348D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.39

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7873, after 0.7512

Leave Link 502 at Sun Aug 18 14:35:29 2019, MaxMem= 2013265920 cpu: 1556.3

(Enter /home/kira/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

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

GePol: Maximum number of non-zero 1st derivatives = 183

Leave Link 701 at Sun Aug 18 14:35:46 2019, MaxMem= 2013265920 cpu: 137.7

(Enter /home/kira/g09/l702.exe)

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

Leave Link 702 at Sun Aug 18 14:35:46 2019, MaxMem= 2013265920 cpu: 0.2

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

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

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

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Sun Aug 18 14:36:25 2019, MaxMem= 2013265920 cpu: 309.6

(Enter /home/kira/g09/l716.exe)

Dipole =-2.62270716D-13 3.39284156D-13-2.15986944D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000017812 -0.000006443 0.000007591

2 6 0.000094790 0.000017353 -0.000002418

3 7 -0.000000000 0.000047176 -0.000010307

4 6 -0.000094790 0.000017353 -0.000002418

5 6 0.000017812 -0.000006443 0.000007591

6 6 0.000008403 0.000000173 -0.000007421

7 6 0.000026792 0.000009928 -0.000087187

8 7 0.000012761 -0.000000000 0.000093755

9 6 0.000026792 -0.000009928 -0.000087187

10 6 0.000004090 0.000005760 0.000022281

11 6 0.000004090 -0.000005760 0.000022281

12 6 -0.000008403 0.000000173 -0.000007421

13 6 -0.000026792 0.000009928 -0.000087187

14 6 -0.000004090 -0.000005760 0.000022281

15 6 -0.000004090 0.000005760 0.000022281

16 6 -0.000026792 -0.000009928 -0.000087187

17 7 -0.000012761 0.000000000 0.000093755

18 6 -0.000008403 -0.000000173 -0.000007421

19 6 0.000094790 -0.000017353 -0.000002418

20 6 -0.000017812 0.000006443 0.000007591

21 6 0.000017812 0.000006443 0.000007591

22 6 -0.000094790 -0.000017353 -0.000002418

23 7 0.000000000 -0.000047176 -0.000010307

24 6 0.000008403 -0.000000173 -0.000007421

25 6 0.000045038 0.000041377 -0.000007785

26 6 -0.000015194 -0.000006997 -0.000014369

27 6 0.000004673 -0.000001010 0.000004821

28 6 -0.000005840 -0.000012914 0.000002580

29 6 0.000002800 0.000009332 -0.000003294

30 6 -0.000018650 -0.000031657 0.000018690

31 6 0.000005840 -0.000012914 0.000002580

32 6 -0.000004673 -0.000001010 0.000004821

33 6 0.000015194 -0.000006997 -0.000014369

34 6 -0.000045038 0.000041377 -0.000007785

35 6 0.000018650 -0.000031657 0.000018690

36 6 -0.000002800 0.000009332 -0.000003294

37 6 0.000045038 -0.000041377 -0.000007785

38 6 -0.000018650 0.000031657 0.000018690

39 6 0.000002800 -0.000009332 -0.000003294

40 6 -0.000005840 0.000012914 0.000002580

41 6 0.000004673 0.000001010 0.000004821

42 6 -0.000015194 0.000006997 -0.000014369

43 6 -0.000045038 -0.000041377 -0.000007785

44 6 0.000018650 0.000031657 0.000018690

45 6 -0.000002800 -0.000009332 -0.000003294

46 6 0.000005840 0.000012914 0.000002580

47 6 -0.000004673 0.000001010 0.000004821

48 6 0.000015194 0.000006997 -0.000014369

49 1 -0.000000385 -0.000009555 0.000000582

50 1 0.000000385 -0.000009555 0.000000582

51 1 -0.000009183 -0.000003769 0.000001090

52 1 -0.000009183 0.000003769 0.000001090

53 1 0.000009183 0.000003769 0.000001090

54 1 0.000009183 -0.000003769 0.000001090

55 1 -0.000000385 0.000009555 0.000000582

56 1 0.000000385 0.000009555 0.000000582

57 1 0.000000888 0.000000051 0.000001372

58 1 0.000000532 -0.000002539 -0.000000061

59 1 -0.000001504 0.000000405 0.000001132

60 1 -0.000001119 -0.000000283 -0.000000961

61 1 0.000000661 0.000000521 -0.000005391

62 1 0.000001504 0.000000405 0.000001132

63 1 -0.000000532 -0.000002539 -0.000000061

64 1 -0.000000888 0.000000051 0.000001372

65 1 -0.000000661 0.000000521 -0.000005391

66 1 0.000001119 -0.000000283 -0.000000961

67 1 0.000000661 -0.000000521 -0.000005391

68 1 -0.000001119 0.000000283 -0.000000961

69 1 -0.000001504 -0.000000405 0.000001132

70 1 0.000000532 0.000002539 -0.000000061

71 1 0.000000888 -0.000000051 0.000001372

72 1 -0.000000661 -0.000000521 -0.000005391

73 1 0.000001119 0.000000283 -0.000000961

74 1 0.000001504 -0.000000405 0.000001132

75 1 -0.000000532 0.000002539 -0.000000061

76 1 -0.000000888 -0.000000051 0.000001372

77 1 -0.000000000 -0.000056727 0.000054049

78 1 -0.000000000 0.000056727 0.000054049

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

Cartesian Forces: Max 0.000094790 RMS 0.000024141

Leave Link 716 at Sun Aug 18 14:36:25 2019, MaxMem= 2013265920 cpu: 0.2

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

Internal Forces: Max 0.000049050 RMS 0.000012925

Search for a local minimum.

Step number 9 out of a maximum of 452

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

RMS Force = .12925D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 3 4 5 6 7

8 9

DE= -1.53D-06 DEPred=-1.46D-06 R= 1.05D+00

TightC=F SS= 1.41D+00 RLast= 1.14D-02 DXNew= 1.3414D+00 3.4100D-02

Trust test= 1.05D+00 RLast= 1.14D-02 DXMaxT set to 7.98D-01

ITU= 1 1 1 1 -1 1 1 1 0

Eigenvalues --- 0.00645 0.00861 0.00861 0.00861 0.01092

Eigenvalues --- 0.01653 0.01669 0.01671 0.01685 0.01689

Eigenvalues --- 0.01698 0.01710 0.01710 0.01710 0.01722

Eigenvalues --- 0.01733 0.01744 0.01830 0.01854 0.01857

Eigenvalues --- 0.01869 0.01909 0.01910 0.01912 0.01915

Eigenvalues --- 0.01950 0.01989 0.02007 0.02013 0.02021

Eigenvalues --- 0.02031 0.02042 0.02057 0.02081 0.02087

Eigenvalues --- 0.02098 0.02099 0.02099 0.02099 0.02101

Eigenvalues --- 0.02115 0.02132 0.02132 0.02132 0.02141

Eigenvalues --- 0.02141 0.02141 0.02141 0.02161 0.02161

Eigenvalues --- 0.02161 0.02165 0.02165 0.02165 0.02165

Eigenvalues --- 0.02166 0.02171 0.02171 0.02171 0.02171

Eigenvalues --- 0.02175 0.02175 0.02175 0.02176 0.02176

Eigenvalues --- 0.02176 0.02176 0.02207 0.02213 0.02217

Eigenvalues --- 0.02225 0.02233 0.02942 0.03194 0.04793

Eigenvalues --- 0.15613 0.15984 0.15984 0.15988 0.15988

Eigenvalues --- 0.15989 0.15991 0.15993 0.15993 0.15993

Eigenvalues --- 0.15993 0.15994 0.15994 0.15994 0.15999

Eigenvalues --- 0.15999 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16008 0.16038 0.16169

Eigenvalues --- 0.21999 0.21999 0.21999 0.22000 0.22000

Eigenvalues --- 0.22000 0.22002 0.22010 0.22483 0.22721

Eigenvalues --- 0.22783 0.22792 0.22796 0.23475 0.23475

Eigenvalues --- 0.23475 0.23529 0.23616 0.23642 0.24149

Eigenvalues --- 0.24509 0.24698 0.24730 0.24767 0.24992

Eigenvalues --- 0.24993 0.24993 0.24997 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25014

Eigenvalues --- 0.26106 0.27958 0.32649 0.33146 0.33146

Eigenvalues --- 0.33146 0.34568 0.34598 0.35400 0.35400

Eigenvalues --- 0.35400 0.35400 0.35400 0.35400 0.35400

Eigenvalues --- 0.35405 0.35405 0.35405 0.35405 0.35417

Eigenvalues --- 0.35452 0.35452 0.35452 0.35461 0.35461

Eigenvalues --- 0.35461 0.35462 0.35564 0.36108 0.36108

Eigenvalues --- 0.36108 0.36171 0.36232 0.36232 0.36232

Eigenvalues --- 0.36298 0.36768 0.36873 0.37380 0.37408

Eigenvalues --- 0.38428 0.39523 0.41119 0.41998 0.41998

Eigenvalues --- 0.41998 0.42160 0.42160 0.42160 0.42169

Eigenvalues --- 0.42587 0.43248 0.43482 0.44372 0.44413

Eigenvalues --- 0.44851 0.45309 0.45484 0.45529 0.45537

Eigenvalues --- 0.45632 0.45856 0.45856 0.45856 0.45863

Eigenvalues --- 0.46150 0.46150 0.46150 0.46271 0.46349

Eigenvalues --- 0.46645 0.46645 0.46645 0.46645 0.46834

Eigenvalues --- 0.46834 0.46834 0.47156 0.47516 0.47806

Eigenvalues --- 0.48571 0.48626 0.49734 0.49854 0.50644

Eigenvalues --- 0.52674 0.53076 0.55329

En-DIIS/RFO-DIIS IScMMF= 0 using points: 9 8 7 6 5

RFO step: Lambda=-2.43527548D-07.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 3.06D-04 SmlDif= 1.00D-05

RMS Error= 0.5487468381D-04 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.09344 -0.05299 -0.04237 0.01183 -0.00992

Iteration 1 RMS(Cart)= 0.00148892 RMS(Int)= 0.00000088

Iteration 2 RMS(Cart)= 0.00000097 RMS(Int)= 0.00000062

ITry= 1 IFail=0 DXMaxC= 6.92D-03 DCOld= 1.00D+10 DXMaxT= 7.98D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 7.58D-09 for atom 69.

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

(Linear) (Quad) (Total)

R1 2.69513 -0.00002 0.00007 -0.00001 0.00006 2.69518

R2 2.59651 -0.00000 -0.00008 -0.00003 -0.00012 2.59639

R3 2.03623 -0.00001 0.00000 -0.00003 -0.00002 2.03620

R4 2.59010 -0.00002 0.00001 -0.00005 -0.00004 2.59005

R5 2.67150 0.00005 -0.00008 0.00006 -0.00002 2.67148

R6 2.59010 -0.00002 0.00001 -0.00005 -0.00004 2.59005

R7 1.91007 0.00004 0.00004 0.00020 0.00024 1.91031

R8 2.69513 -0.00002 0.00007 -0.00001 0.00006 2.69518

R9 2.67150 0.00005 -0.00008 0.00006 -0.00002 2.67148

R10 2.03623 -0.00001 0.00000 -0.00003 -0.00002 2.03620

R11 2.66615 0.00000 -0.00001 -0.00005 -0.00005 2.66610

R12 2.79791 0.00001 0.00003 0.00010 0.00013 2.79804

R13 2.58136 -0.00000 -0.00004 -0.00004 -0.00008 2.58128

R14 2.74990 -0.00001 0.00002 -0.00003 -0.00001 2.74989

R15 2.58136 -0.00000 -0.00004 -0.00004 -0.00008 2.58128

R16 2.74990 -0.00001 0.00002 -0.00003 -0.00001 2.74989

R17 2.66615 0.00000 -0.00001 -0.00005 -0.00005 2.66610

R18 2.56226 0.00000 -0.00000 0.00003 0.00003 2.56229

R19 2.03825 -0.00000 0.00000 -0.00001 -0.00001 2.03824

R20 2.03825 -0.00000 0.00000 -0.00001 -0.00001 2.03824

R21 2.66615 0.00000 -0.00001 -0.00005 -0.00005 2.66610

R22 2.79791 0.00001 0.00003 0.00010 0.00013 2.79804

R23 2.74990 -0.00001 0.00002 -0.00003 -0.00001 2.74989

R24 2.58136 -0.00000 -0.00004 -0.00004 -0.00008 2.58128

R25 2.56226 0.00000 -0.00000 0.00003 0.00003 2.56229

R26 2.03825 -0.00000 0.00000 -0.00001 -0.00001 2.03824

R27 2.74990 -0.00001 0.00002 -0.00003 -0.00001 2.74989

R28 2.03825 -0.00000 0.00000 -0.00001 -0.00001 2.03824

R29 2.58136 -0.00000 -0.00004 -0.00004 -0.00008 2.58128

R30 2.66615 0.00000 -0.00001 -0.00005 -0.00005 2.66610

R31 2.67150 0.00005 -0.00008 0.00006 -0.00002 2.67148

R32 2.79791 0.00001 0.00003 0.00010 0.00013 2.79804

R33 2.69513 -0.00002 0.00007 -0.00001 0.00006 2.69518

R34 2.59010 -0.00002 0.00001 -0.00005 -0.00004 2.59005

R35 2.59651 -0.00000 -0.00008 -0.00003 -0.00012 2.59639

R36 2.03623 -0.00001 0.00000 -0.00003 -0.00002 2.03620

R37 2.69513 -0.00002 0.00007 -0.00001 0.00006 2.69518

R38 2.03623 -0.00001 0.00000 -0.00003 -0.00002 2.03620

R39 2.59010 -0.00002 0.00001 -0.00005 -0.00004 2.59005

R40 2.67150 0.00005 -0.00008 0.00006 -0.00002 2.67148

R41 1.91007 0.00004 0.00004 0.00020 0.00024 1.91031

R42 2.79791 0.00001 0.00003 0.00010 0.00013 2.79804

R43 2.65126 -0.00001 -0.00001 -0.00005 -0.00007 2.65120

R44 2.65120 -0.00001 -0.00002 -0.00007 -0.00009 2.65111

R45 2.62814 -0.00000 0.00000 0.00001 0.00002 2.62815

R46 2.04814 -0.00000 0.00001 -0.00000 0.00000 2.04814

R47 2.63516 0.00000 0.00000 -0.00000 -0.00000 2.63516

R48 2.04947 -0.00000 0.00000 -0.00000 -0.00000 2.04946

R49 2.63562 -0.00001 -0.00000 -0.00002 -0.00002 2.63560

R50 2.04976 -0.00000 -0.00000 -0.00000 -0.00000 2.04976

R51 2.62759 -0.00000 0.00000 0.00002 0.00002 2.62761

R52 2.04948 -0.00000 0.00000 -0.00000 0.00000 2.04948

R53 2.04790 -0.00000 0.00001 -0.00000 0.00000 2.04790

R54 2.63516 0.00000 0.00000 -0.00000 -0.00000 2.63516

R55 2.63562 -0.00001 -0.00000 -0.00002 -0.00002 2.63560

R56 2.04976 -0.00000 -0.00000 -0.00000 -0.00000 2.04976

R57 2.62814 -0.00000 0.00000 0.00001 0.00002 2.62815

R58 2.04947 -0.00000 0.00000 -0.00000 -0.00000 2.04946

R59 2.65126 -0.00001 -0.00001 -0.00005 -0.00007 2.65120

R60 2.04814 -0.00000 0.00001 -0.00000 0.00000 2.04814

R61 2.65120 -0.00001 -0.00002 -0.00007 -0.00009 2.65111

R62 2.62759 -0.00000 0.00000 0.00002 0.00002 2.62761

R63 2.04790 -0.00000 0.00001 -0.00000 0.00000 2.04790

R64 2.04948 -0.00000 0.00000 -0.00000 0.00000 2.04948

R65 2.65120 -0.00001 -0.00002 -0.00007 -0.00009 2.65111

R66 2.65126 -0.00001 -0.00001 -0.00005 -0.00007 2.65120

R67 2.62759 -0.00000 0.00000 0.00002 0.00002 2.62761

R68 2.04790 -0.00000 0.00001 -0.00000 0.00000 2.04790

R69 2.63562 -0.00001 -0.00000 -0.00002 -0.00002 2.63560

R70 2.04948 -0.00000 0.00000 -0.00000 0.00000 2.04948

R71 2.63516 0.00000 0.00000 -0.00000 -0.00000 2.63516

R72 2.04976 -0.00000 -0.00000 -0.00000 -0.00000 2.04976

R73 2.62814 -0.00000 0.00000 0.00001 0.00002 2.62815

R74 2.04947 -0.00000 0.00000 -0.00000 -0.00000 2.04946

R75 2.04814 -0.00000 0.00001 -0.00000 0.00000 2.04814

R76 2.65120 -0.00001 -0.00002 -0.00007 -0.00009 2.65111

R77 2.65126 -0.00001 -0.00001 -0.00005 -0.00007 2.65120

R78 2.62759 -0.00000 0.00000 0.00002 0.00002 2.62761

R79 2.04790 -0.00000 0.00001 -0.00000 0.00000 2.04790

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A3 2.21686 0.00001 0.00004 0.00013 0.00017 2.21703

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A9 2.17865 0.00001 0.00000 0.00004 0.00004 2.17869

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A19 2.18354 -0.00002 -0.00001 -0.00008 -0.00009 2.18345

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A23 1.93446 0.00000 0.00002 0.00002 0.00004 1.93451

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A72 2.10018 -0.00002 -0.00001 -0.00014 -0.00014 2.10003

A73 2.08723 0.00001 0.00001 0.00006 0.00007 2.08730

A74 2.09541 0.00001 -0.00000 0.00008 0.00007 2.09549

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A76 2.08874 -0.00000 -0.00000 0.00000 -0.00000 2.08874

A77 2.09735 0.00000 0.00001 -0.00000 0.00001 2.09736

A78 2.09246 0.00001 0.00000 0.00007 0.00007 2.09253

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D2 -3.10157 0.00001 0.00010 0.00050 0.00060 -3.10097

D3 -3.09385 0.00001 -0.00009 0.00033 0.00024 -3.09361

D4 0.06629 0.00000 0.00011 0.00030 0.00041 0.06669

D5 0.00000 -0.00000 -0.00000 0.00000 0.00000 0.00000

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D7 3.11467 0.00001 -0.00000 0.00020 0.00019 3.11486

D8 -0.00000 0.00000 -0.00000 -0.00000 0.00000 0.00000

D9 -0.03579 -0.00002 0.00015 -0.00087 -0.00072 -0.03651

D10 3.09641 -0.00003 -0.00013 -0.00189 -0.00202 3.09439

D11 3.08744 -0.00002 -0.00004 -0.00085 -0.00089 3.08655

D12 -0.06355 -0.00002 -0.00032 -0.00186 -0.00218 -0.06573

D13 -2.97587 -0.00001 -0.00029 -0.00115 -0.00144 -2.97731

D14 0.16089 -0.00001 -0.00031 -0.00141 -0.00172 0.15917

D15 0.18769 -0.00001 -0.00006 -0.00118 -0.00124 0.18645

D16 -2.95873 -0.00002 -0.00008 -0.00144 -0.00152 -2.96025

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D18 -3.08744 0.00002 0.00004 0.00085 0.00089 -3.08655

D19 -3.09641 0.00003 0.00013 0.00189 0.00202 -3.09439

D20 0.06355 0.00002 0.00032 0.00186 0.00218 0.06573

D21 -0.02147 -0.00001 0.00009 -0.00052 -0.00043 -0.02191

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D27 2.97587 0.00001 0.00029 0.00115 0.00144 2.97731

D28 -0.16089 0.00001 0.00031 0.00141 0.00172 -0.15917

D29 -0.18247 -0.00001 -0.00008 -0.00012 -0.00021 -0.18268

D30 2.98466 0.00001 0.00001 0.00051 0.00052 2.98518

D31 2.95422 -0.00002 -0.00010 -0.00039 -0.00049 2.95373

D32 -0.16183 0.00000 -0.00001 0.00024 0.00024 -0.16159

D33 -0.96858 -0.00001 -0.00031 -0.00091 -0.00121 -0.96980

D34 2.17236 -0.00001 -0.00033 -0.00070 -0.00103 2.17133

D35 2.17750 -0.00000 -0.00029 -0.00066 -0.00095 2.17655

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D38 0.04497 -0.00003 0.00006 -0.00052 -0.00046 0.04451

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D40 -0.08051 -0.00001 -0.00011 -0.00021 -0.00032 -0.08083

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D59 0.16183 -0.00000 0.00001 -0.00024 -0.00024 0.16159

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D61 0.96858 0.00001 0.00031 0.00091 0.00121 0.96980

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D69 3.07397 0.00001 -0.00014 -0.00004 -0.00018 3.07379

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D73 3.11119 -0.00001 0.00001 0.00001 0.00002 3.11121

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D78 -0.08051 -0.00001 -0.00011 -0.00021 -0.00032 -0.08083

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D81 2.98466 0.00001 0.00001 0.00051 0.00052 2.98518

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D83 -0.18247 -0.00001 -0.00008 -0.00012 -0.00021 -0.18268

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D101 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

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D107 -3.09385 0.00001 -0.00009 0.00033 0.00024 -3.09361

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D133 0.00917 0.00000 0.00001 0.00008 0.00008 0.00926

D134 -3.13233 0.00000 -0.00000 0.00002 0.00002 -3.13231

D135 -3.13242 0.00000 -0.00001 0.00012 0.00011 -3.13230

D136 0.00927 0.00000 -0.00002 0.00007 0.00005 0.00931

D137 0.00928 -0.00000 -0.00001 -0.00007 -0.00008 0.00920

D138 -3.13222 -0.00000 -0.00003 -0.00010 -0.00013 -3.13235

D139 -3.13240 -0.00000 -0.00000 -0.00001 -0.00002 -3.13242

D140 0.00928 -0.00000 -0.00002 -0.00004 -0.00007 0.00922

D141 -0.01821 -0.00000 0.00000 -0.00006 -0.00006 -0.01827

D142 -3.13163 -0.00000 0.00000 -0.00018 -0.00018 -3.13180

D143 3.12329 -0.00000 0.00002 -0.00003 -0.00000 3.12328

D144 0.00987 -0.00000 0.00002 -0.00015 -0.00013 0.00975

D145 -0.00917 -0.00000 -0.00001 -0.00008 -0.00008 -0.00926

D146 3.13242 -0.00000 0.00001 -0.00012 -0.00011 3.13230

D147 3.13233 -0.00000 0.00000 -0.00002 -0.00002 3.13231

D148 -0.00927 -0.00000 0.00002 -0.00007 -0.00005 -0.00931

D149 -0.00928 0.00000 0.00001 0.00007 0.00008 -0.00920

D150 3.13222 0.00000 0.00003 0.00010 0.00013 3.13235

D151 3.13240 0.00000 0.00000 0.00001 0.00002 3.13242

D152 -0.00928 0.00000 0.00002 0.00004 0.00007 -0.00922

D153 0.01872 0.00000 -0.00001 -0.00005 -0.00005 0.01867

D154 3.13126 0.00000 -0.00000 0.00003 0.00002 3.13128

D155 -3.12287 0.00000 -0.00002 -0.00000 -0.00003 -3.12289

D156 -0.01033 0.00000 -0.00002 0.00007 0.00005 -0.01028

D157 3.13245 -0.00000 0.00004 -0.00003 0.00001 3.13246

D158 -0.00978 0.00000 0.00002 0.00017 0.00019 -0.00959

D159 0.01977 -0.00000 0.00003 -0.00010 -0.00007 0.01971

D160 -3.12246 0.00000 0.00001 0.00010 0.00011 -3.12235

D161 3.13229 -0.00000 -0.00003 0.00002 -0.00001 3.13228

D162 0.01871 -0.00000 -0.00003 -0.00010 -0.00013 0.01858

D163 -0.00867 -0.00000 -0.00001 -0.00018 -0.00019 -0.00886

D164 -3.12224 -0.00000 -0.00001 -0.00030 -0.00031 -3.12255

D165 0.01821 0.00000 -0.00000 0.00006 0.00006 0.01827

D166 -3.12329 0.00000 -0.00002 0.00003 0.00000 -3.12328

D167 3.13163 0.00000 -0.00000 0.00018 0.00018 3.13180

D168 -0.00987 0.00000 -0.00002 0.00015 0.00013 -0.00975

D169 3.13229 -0.00000 -0.00003 0.00002 -0.00001 3.13228

D170 0.01871 -0.00000 -0.00003 -0.00010 -0.00013 0.01858

D171 -0.00867 -0.00000 -0.00001 -0.00018 -0.00019 -0.00886

D172 -3.12224 -0.00000 -0.00001 -0.00030 -0.00031 -3.12255

D173 3.13245 -0.00000 0.00004 -0.00003 0.00001 3.13246

D174 0.01977 -0.00000 0.00003 -0.00010 -0.00007 0.01971

D175 -0.00978 0.00000 0.00002 0.00017 0.00019 -0.00959

D176 -3.12246 0.00000 0.00001 0.00010 0.00011 -3.12235

D177 0.01821 0.00000 -0.00000 0.00006 0.00006 0.01827

D178 -3.12329 0.00000 -0.00002 0.00003 0.00000 -3.12328

D179 3.13163 0.00000 -0.00000 0.00018 0.00018 3.13180

D180 -0.00987 0.00000 -0.00002 0.00015 0.00013 -0.00975

D181 -0.00928 0.00000 0.00001 0.00007 0.00008 -0.00920

D182 3.13240 0.00000 0.00000 0.00001 0.00002 3.13242

D183 3.13222 0.00000 0.00003 0.00010 0.00013 3.13235

D184 -0.00928 0.00000 0.00002 0.00004 0.00007 -0.00922

D185 -0.00917 -0.00000 -0.00001 -0.00008 -0.00008 -0.00926

D186 3.13242 -0.00000 0.00001 -0.00012 -0.00011 3.13230

D187 3.13233 -0.00000 0.00000 -0.00002 -0.00002 3.13231

D188 -0.00927 -0.00000 0.00002 -0.00007 -0.00005 -0.00931

D189 0.01872 0.00000 -0.00001 -0.00005 -0.00005 0.01867

D190 3.13126 0.00000 -0.00000 0.00003 0.00002 3.13128

D191 -3.12287 0.00000 -0.00002 -0.00000 -0.00003 -3.12289

D192 -0.01033 0.00000 -0.00002 0.00007 0.00005 -0.01028

D193 -3.13229 0.00000 0.00003 -0.00002 0.00001 -3.13228

D194 -0.01871 0.00000 0.00003 0.00010 0.00013 -0.01858

D195 0.00867 0.00000 0.00001 0.00018 0.00019 0.00886

D196 3.12224 0.00000 0.00001 0.00030 0.00031 3.12255

D197 -3.13245 0.00000 -0.00004 0.00003 -0.00001 -3.13246

D198 -0.01977 0.00000 -0.00003 0.00010 0.00007 -0.01971

D199 0.00978 -0.00000 -0.00002 -0.00017 -0.00019 0.00959

D200 3.12246 -0.00000 -0.00001 -0.00010 -0.00011 3.12235

D201 -0.01821 -0.00000 0.00000 -0.00006 -0.00006 -0.01827

D202 3.12329 -0.00000 0.00002 -0.00003 -0.00000 3.12328

D203 -3.13163 -0.00000 0.00000 -0.00018 -0.00018 -3.13180

D204 0.00987 -0.00000 0.00002 -0.00015 -0.00013 0.00975

D205 0.00928 -0.00000 -0.00001 -0.00007 -0.00008 0.00920

D206 -3.13240 -0.00000 -0.00000 -0.00001 -0.00002 -3.13242

D207 -3.13222 -0.00000 -0.00003 -0.00010 -0.00013 -3.13235

D208 0.00928 -0.00000 -0.00002 -0.00004 -0.00007 0.00922

D209 0.00917 0.00000 0.00001 0.00008 0.00008 0.00926

D210 -3.13242 0.00000 -0.00001 0.00012 0.00011 -3.13230

D211 -3.13233 0.00000 -0.00000 0.00002 0.00002 -3.13231

D212 0.00927 0.00000 -0.00002 0.00007 0.00005 0.00931

D213 -0.01872 -0.00000 0.00001 0.00005 0.00005 -0.01867

D214 -3.13126 -0.00000 0.00000 -0.00003 -0.00002 -3.13128

D215 3.12287 -0.00000 0.00002 0.00000 0.00003 3.12289

D216 0.01033 -0.00000 0.00002 -0.00007 -0.00005 0.01028

Item Value Threshold Converged?

Maximum Force 0.000049 0.000450 YES

RMS Force 0.000013 0.000300 YES

Maximum Displacement 0.006923 0.001800 NO

RMS Displacement 0.001489 0.001200 NO

Predicted change in Energy=-6.643186D-07

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Aug 18 14:36:25 2019, MaxMem= 2013265920 cpu: 1.3

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

Stoichiometry C44H30N4(1+,2)

Framework group C2V[SGV(H2N2),SGV'(N2),X(C44H28)]

Deg. of freedom 59

Full point group C2V NOp 4

RotChk: IX=0 Diff= 7.46D-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 -0.686976 4.173391 0.508033

2 6 0 -1.125038 2.863317 0.153157

3 7 0 0.000000 2.100715 -0.023658

4 6 0 1.125038 2.863317 0.153157

5 6 0 0.686976 4.173391 0.508033

6 6 0 2.460643 2.430315 -0.011692

7 6 0 2.860728 1.087659 -0.178055

8 7 0 2.052997 -0.000000 -0.003699

9 6 0 2.860728 -1.087659 -0.178055

10 6 0 4.211549 -0.677953 -0.531554

11 6 0 4.211549 0.677953 -0.531554

12 6 0 -2.460643 2.430315 -0.011692

13 6 0 -2.860728 1.087659 -0.178055

14 6 0 -4.211549 0.677953 -0.531554

15 6 0 -4.211549 -0.677953 -0.531554

16 6 0 -2.860728 -1.087659 -0.178055

17 7 0 -2.052997 0.000000 -0.003699

18 6 0 -2.460643 -2.430315 -0.011692

19 6 0 -1.125038 -2.863317 0.153157

20 6 0 -0.686976 -4.173391 0.508033

21 6 0 0.686976 -4.173391 0.508033

22 6 0 1.125038 -2.863317 0.153157

23 7 0 -0.000000 -2.100715 -0.023658

24 6 0 2.460643 -2.430315 -0.011692

25 6 0 3.507012 3.477851 -0.000280

26 6 0 3.443300 4.560918 -0.889765

27 6 0 4.435149 5.535789 -0.881267

28 6 0 5.489297 5.454669 0.027976

29 6 0 5.554430 4.387244 0.923266

30 6 0 4.576893 3.398581 0.903725

31 6 0 -5.489297 5.454669 0.027976

32 6 0 -4.435149 5.535789 -0.881267

33 6 0 -3.443300 4.560918 -0.889765

34 6 0 -3.507012 3.477851 -0.000280

35 6 0 -4.576893 3.398581 0.903725

36 6 0 -5.554430 4.387244 0.923266

37 6 0 3.507012 -3.477851 -0.000280

38 6 0 4.576893 -3.398581 0.903725

39 6 0 5.554430 -4.387244 0.923266

40 6 0 5.489297 -5.454669 0.027976

41 6 0 4.435149 -5.535789 -0.881267

42 6 0 3.443300 -4.560918 -0.889765

43 6 0 -3.507012 -3.477851 -0.000280

44 6 0 -4.576893 -3.398581 0.903725

45 6 0 -5.554430 -4.387244 0.923266

46 6 0 -5.489297 -5.454669 0.027976

47 6 0 -4.435149 -5.535789 -0.881267

48 6 0 -3.443300 -4.560918 -0.889765

49 1 0 -1.335838 4.997399 0.755062

50 1 0 1.335838 4.997399 0.755062

51 1 0 5.031487 -1.335811 -0.772966

52 1 0 5.031487 1.335811 -0.772966

53 1 0 -5.031487 1.335811 -0.772966

54 1 0 -5.031487 -1.335811 -0.772966

55 1 0 -1.335838 -4.997399 0.755062

56 1 0 1.335838 -4.997399 0.755062

57 1 0 2.629785 4.620261 -1.603460

58 1 0 4.384697 6.359262 -1.585220

59 1 0 6.257368 6.220495 0.038958

60 1 0 6.367661 4.324289 1.638048

61 1 0 4.623233 2.574297 1.605736

62 1 0 -6.257368 6.220495 0.038958

63 1 0 -4.384697 6.359262 -1.585220

64 1 0 -2.629785 4.620261 -1.603460

65 1 0 -4.623233 2.574297 1.605736

66 1 0 -6.367661 4.324289 1.638048

67 1 0 4.623233 -2.574297 1.605736

68 1 0 6.367661 -4.324289 1.638048

69 1 0 6.257368 -6.220495 0.038958

70 1 0 4.384697 -6.359262 -1.585220

71 1 0 2.629785 -4.620261 -1.603460

72 1 0 -4.623233 -2.574297 1.605736

73 1 0 -6.367661 -4.324289 1.638048

74 1 0 -6.257368 -6.220495 0.038958

75 1 0 -4.384697 -6.359262 -1.585220

76 1 0 -2.629785 -4.620261 -1.603460

77 1 0 0.000000 1.113981 -0.243331

78 1 0 -0.000000 -1.113981 -0.243331

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

Rotational constants (GHZ): 0.0593157 0.0585922 0.0302906

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

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

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

There are 261 symmetry adapted cartesian basis functions of A1 symmetry.

There are 240 symmetry adapted cartesian basis functions of A2 symmetry.

There are 249 symmetry adapted cartesian basis functions of B1 symmetry.

There are 252 symmetry adapted cartesian basis functions of B2 symmetry.

There are 248 symmetry adapted basis functions of A1 symmetry.

There are 229 symmetry adapted basis functions of A2 symmetry.

There are 237 symmetry adapted basis functions of B1 symmetry.

There are 240 symmetry adapted basis functions of B2 symmetry.

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

161 alpha electrons 160 beta electrons

nuclear repulsion energy 5372.2283108355 Hartrees.

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

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

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

NAtoms= 78 NActive= 78 NUniq= 21 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=T Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2128271945 Hartrees.

Nuclear repulsion after empirical dispersion term = 5372.0154836410 Hartrees.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 78

GePol: Total number of spheres = 78

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

GePol: Number of points = 5702

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.16D-08

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 290

GePol: Fraction of low-weight points (<1% of avg) = 5.09%

GePol: Cavity surface area = 608.647 Ang\*\*2

GePol: Cavity volume = 626.229 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0022217381 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5372.0132619030 Hartrees.

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(Enter /home/kira/g09/l302.exe)

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

NBasis= 954 RedAO= T EigKep= 6.36D-05 NBF= 248 229 237 240

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 248 229 237 240

Precomputing XC quadrature grid using

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

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

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

Leave Link 302 at Sun Aug 18 14:36:26 2019, MaxMem= 2013265920 cpu: 9.7

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

DipDrv: MaxL=1.

Leave Link 303 at Sun Aug 18 14:36:27 2019, MaxMem= 2013265920 cpu: 1.2

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

Initial guess from the checkpoint file: "TPPcation.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) (B1) (A1) (B2) (A2) (A1) (B1) (A2) (B2)

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

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The electronic state of the initial guess is 2-A1.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7873 S= 0.5185

Leave Link 401 at Sun Aug 18 14:36:31 2019, MaxMem= 2013265920 cpu: 34.8

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3049894 IEndB= 3049894 NGot= 2013265920 MDV= 2011237673

LenX= 2011237673 LenY= 2010232667

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

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

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

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

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

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 97538412.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.44D-15 for 5697.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.59D-15 for 3564 342.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.00D-15 for 5697.

Iteration 1 A^-1\*A deviation from orthogonality is 3.10D-12 for 4540 4535.

E= -1914.20122814589

DIIS: error= 1.22D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.20122814589 IErMin= 1 ErrMin= 1.22D-04

ErrMax= 1.22D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.85D-05 BMatP= 2.85D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.22D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.503 Goal= None Shift= 0.000

Gap= 0.515 Goal= None Shift= 0.000

RMSDP=4.64D-06 MaxDP=1.90D-04 OVMax= 6.28D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.64D-06 CP: 1.00D+00

E= -1914.20124090124 Delta-E= -0.000012755344 Rises=F Damp=F

DIIS: error= 1.38D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.20124090124 IErMin= 2 ErrMin= 1.38D-05

ErrMax= 1.38D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.88D-07 BMatP= 2.85D-05

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

Coeff-Com: -0.471D-01 0.105D+01

Coeff: -0.471D-01 0.105D+01

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=9.00D-07 MaxDP=4.50D-05 DE=-1.28D-05 OVMax= 2.03D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 8.76D-07 CP: 1.00D+00 1.04D+00

E= -1914.20124098561 Delta-E= -0.000000084377 Rises=F Damp=F

DIIS: error= 1.81D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.20124098561 IErMin= 2 ErrMin= 1.38D-05

ErrMax= 1.81D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.19D-07 BMatP= 4.88D-07

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

Coeff-Com: -0.376D-01 0.586D+00 0.452D+00

Coeff: -0.376D-01 0.586D+00 0.452D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=5.62D-07 MaxDP=4.23D-05 DE=-8.44D-08 OVMax= 1.82D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 3.42D-07 CP: 1.00D+00 1.06D+00 5.05D-01

E= -1914.20124110978 Delta-E= -0.000000124167 Rises=F Damp=F

DIIS: error= 6.57D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.20124110978 IErMin= 4 ErrMin= 6.57D-06

ErrMax= 6.57D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.60D-08 BMatP= 4.88D-07

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

Coeff-Com: -0.131D-01 0.157D+00 0.271D+00 0.585D+00

Coeff: -0.131D-01 0.157D+00 0.271D+00 0.585D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=1.79D-07 MaxDP=1.47D-05 DE=-1.24D-07 OVMax= 6.79D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 9.95D-08 CP: 1.00D+00 1.06D+00 6.21D-01 6.83D-01

E= -1914.20124112627 Delta-E= -0.000000016494 Rises=F Damp=F

DIIS: error= 1.23D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.20124112627 IErMin= 5 ErrMin= 1.23D-06

ErrMax= 1.23D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.02D-09 BMatP= 7.60D-08

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

Coeff-Com: -0.318D-02 0.271D-01 0.887D-01 0.265D+00 0.622D+00

Coeff: -0.318D-02 0.271D-01 0.887D-01 0.265D+00 0.622D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=4.85D-08 MaxDP=2.94D-06 DE=-1.65D-08 OVMax= 1.20D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.51D-08 CP: 1.00D+00 1.06D+00 6.12D-01 7.54D-01 8.00D-01

E= -1914.20124112716 Delta-E= -0.000000000881 Rises=F Damp=F

DIIS: error= 6.80D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.20124112716 IErMin= 6 ErrMin= 6.80D-07

ErrMax= 6.80D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.10D-09 BMatP= 4.02D-09

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

Coeff-Com: 0.627D-03-0.148D-01-0.131D-02 0.390D-01 0.370D+00 0.607D+00

Coeff: 0.627D-03-0.148D-01-0.131D-02 0.390D-01 0.370D+00 0.607D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=2.02D-08 MaxDP=1.57D-06 DE=-8.81D-10 OVMax= 5.49D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.17D-08 CP: 1.00D+00 1.06D+00 6.23D-01 7.56D-01 8.80D-01

CP: 7.04D-01

E= -1914.20124112741 Delta-E= -0.000000000252 Rises=F Damp=F

DIIS: error= 2.08D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.20124112741 IErMin= 7 ErrMin= 2.08D-07

ErrMax= 2.08D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.05D-10 BMatP= 1.10D-09

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

Coeff-Com: 0.528D-03-0.957D-02-0.598D-02 0.467D-02 0.159D+00 0.334D+00

Coeff-Com: 0.517D+00

Coeff: 0.528D-03-0.957D-02-0.598D-02 0.467D-02 0.159D+00 0.334D+00

Coeff: 0.517D+00

Gap= 0.097 Goal= None Shift= 0.000

Gap= 0.056 Goal= None Shift= 0.000

RMSDP=6.14D-09 MaxDP=4.03D-07 DE=-2.52D-10 OVMax= 2.30D-06

Error on total polarization charges = 0.07902

SCF Done: E(UB3LYP) = -1914.20124113 A.U. after 7 cycles

NFock= 7 Conv=0.61D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7873 S= 0.5185

<L.S>= 0.000000000000E+00

KE= 1.906181753880D+03 PE=-1.515861332392D+04 EE= 5.966217067011D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.39

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7873, after 0.7512

Leave Link 502 at Sun Aug 18 14:39:31 2019, MaxMem= 2013265920 cpu: 1424.3

(Enter /home/kira/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

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

GePol: Maximum number of non-zero 1st derivatives = 182

Leave Link 701 at Sun Aug 18 14:39:48 2019, MaxMem= 2013265920 cpu: 136.6

(Enter /home/kira/g09/l702.exe)

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

Leave Link 702 at Sun Aug 18 14:39:48 2019, MaxMem= 2013265920 cpu: 0.2

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

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

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

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Sun Aug 18 14:40:27 2019, MaxMem= 2013265920 cpu: 308.5

(Enter /home/kira/g09/l716.exe)

Dipole = 8.12425451D-13-3.02868841D-12-2.12539564D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000067722 -0.000024403 -0.000013378

2 6 0.000037844 0.000016357 0.000044026

3 7 -0.000000000 -0.000017006 -0.000091657

4 6 -0.000037844 0.000016357 0.000044026

5 6 0.000067722 -0.000024403 -0.000013378

6 6 0.000026900 0.000012969 0.000017301

7 6 0.000030509 0.000024720 -0.000013936

8 7 -0.000037418 0.000000000 0.000027625

9 6 0.000030509 -0.000024720 -0.000013936

10 6 -0.000011085 0.000017979 0.000001995

11 6 -0.000011085 -0.000017979 0.000001995

12 6 -0.000026900 0.000012969 0.000017301

13 6 -0.000030509 0.000024720 -0.000013936

14 6 0.000011085 -0.000017979 0.000001995

15 6 0.000011085 0.000017979 0.000001995

16 6 -0.000030509 -0.000024720 -0.000013936

17 7 0.000037418 0.000000000 0.000027625

18 6 -0.000026900 -0.000012969 0.000017301

19 6 0.000037844 -0.000016357 0.000044026

20 6 -0.000067722 0.000024403 -0.000013378

21 6 0.000067722 0.000024403 -0.000013378

22 6 -0.000037844 -0.000016357 0.000044026

23 7 0.000000000 0.000017006 -0.000091657

24 6 0.000026900 -0.000012969 0.000017301

25 6 -0.000024660 -0.000001731 -0.000032534

26 6 0.000002448 0.000008055 0.000006730

27 6 0.000000586 -0.000000045 -0.000001319

28 6 0.000004316 -0.000001696 -0.000001276

29 6 0.000001423 -0.000000868 0.000004376

30 6 0.000003586 0.000001288 0.000016412

31 6 -0.000004316 -0.000001696 -0.000001276

32 6 -0.000000586 -0.000000045 -0.000001319

33 6 -0.000002448 0.000008055 0.000006730

34 6 0.000024660 -0.000001731 -0.000032534

35 6 -0.000003586 0.000001288 0.000016412

36 6 -0.000001423 -0.000000868 0.000004376

37 6 -0.000024660 0.000001731 -0.000032534

38 6 0.000003586 -0.000001288 0.000016412

39 6 0.000001423 0.000000868 0.000004376

40 6 0.000004316 0.000001696 -0.000001276

41 6 0.000000586 0.000000045 -0.000001319

42 6 0.000002448 -0.000008055 0.000006730

43 6 0.000024660 0.000001731 -0.000032534

44 6 -0.000003586 -0.000001288 0.000016412

45 6 -0.000001423 0.000000868 0.000004376

46 6 -0.000004316 0.000001696 -0.000001276

47 6 -0.000000586 0.000000045 -0.000001319

48 6 -0.000002448 -0.000008055 0.000006730

49 1 0.000005290 0.000007315 -0.000004054

50 1 -0.000005290 0.000007315 -0.000004054

51 1 -0.000001354 0.000004701 -0.000003628

52 1 -0.000001354 -0.000004701 -0.000003628

53 1 0.000001354 -0.000004701 -0.000003628

54 1 0.000001354 0.000004701 -0.000003628

55 1 0.000005290 -0.000007315 -0.000004054

56 1 -0.000005290 -0.000007315 -0.000004054

57 1 -0.000002751 -0.000002646 0.000006079

58 1 0.000001960 0.000000162 0.000001481

59 1 0.000000141 0.000001645 0.000000408

60 1 0.000000084 0.000001892 -0.000001429

61 1 0.000000838 0.000007367 -0.000003203

62 1 -0.000000141 0.000001645 0.000000408

63 1 -0.000001960 0.000000162 0.000001481

64 1 0.000002751 -0.000002646 0.000006079

65 1 -0.000000838 0.000007367 -0.000003203

66 1 -0.000000084 0.000001892 -0.000001429

67 1 0.000000838 -0.000007367 -0.000003203

68 1 0.000000084 -0.000001892 -0.000001429

69 1 0.000000141 -0.000001645 0.000000408

70 1 0.000001960 -0.000000162 0.000001481

71 1 -0.000002751 0.000002646 0.000006079

72 1 -0.000000838 -0.000007367 -0.000003203

73 1 -0.000000084 -0.000001892 -0.000001429

74 1 -0.000000141 -0.000001645 0.000000408

75 1 -0.000001960 -0.000000162 0.000001481

76 1 0.000002751 0.000002646 0.000006079

77 1 -0.000000000 0.000006990 0.000015929

78 1 -0.000000000 -0.000006990 0.000015929

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

Cartesian Forces: Max 0.000091657 RMS 0.000018645

Leave Link 716 at Sun Aug 18 14:40:27 2019, MaxMem= 2013265920 cpu: 0.2

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

Internal Forces: Max 0.000037849 RMS 0.000009258

Search for a local minimum.

Step number 10 out of a maximum of 452

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .92585D-05 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 3 4 5 6 7

8 9 10

DE= -5.68D-07 DEPred=-6.64D-07 R= 8.54D-01

Trust test= 8.54D-01 RLast= 1.02D-02 DXMaxT set to 7.98D-01

ITU= 0 1 1 1 1 -1 1 1 1 0

Eigenvalues --- 0.00640 0.00861 0.00861 0.00861 0.00891

Eigenvalues --- 0.01653 0.01669 0.01669 0.01671 0.01685

Eigenvalues --- 0.01697 0.01710 0.01710 0.01710 0.01734

Eigenvalues --- 0.01744 0.01756 0.01830 0.01857 0.01858

Eigenvalues --- 0.01869 0.01909 0.01910 0.01912 0.01916

Eigenvalues --- 0.01950 0.02007 0.02013 0.02021 0.02022

Eigenvalues --- 0.02031 0.02042 0.02057 0.02080 0.02086

Eigenvalues --- 0.02098 0.02099 0.02099 0.02099 0.02111

Eigenvalues --- 0.02132 0.02132 0.02132 0.02139 0.02141

Eigenvalues --- 0.02141 0.02141 0.02157 0.02161 0.02161

Eigenvalues --- 0.02161 0.02165 0.02165 0.02165 0.02165

Eigenvalues --- 0.02168 0.02171 0.02171 0.02171 0.02175

Eigenvalues --- 0.02175 0.02175 0.02176 0.02176 0.02176

Eigenvalues --- 0.02176 0.02193 0.02206 0.02213 0.02217

Eigenvalues --- 0.02226 0.02233 0.03072 0.03628 0.04677

Eigenvalues --- 0.15805 0.15984 0.15984 0.15988 0.15988

Eigenvalues --- 0.15991 0.15993 0.15993 0.15993 0.15994

Eigenvalues --- 0.15994 0.15994 0.15994 0.15996 0.15999

Eigenvalues --- 0.15999 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16002 0.16033 0.16038 0.16148

Eigenvalues --- 0.21378 0.21999 0.21999 0.21999 0.22000

Eigenvalues --- 0.22000 0.22000 0.22010 0.22017 0.22721

Eigenvalues --- 0.22783 0.22792 0.22796 0.23475 0.23475

Eigenvalues --- 0.23475 0.23529 0.23637 0.23936 0.24445

Eigenvalues --- 0.24699 0.24735 0.24765 0.24767 0.24992

Eigenvalues --- 0.24993 0.24993 0.24996 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.26030

Eigenvalues --- 0.26467 0.27992 0.32602 0.33146 0.33146

Eigenvalues --- 0.33146 0.34568 0.34598 0.35400 0.35400

Eigenvalues --- 0.35400 0.35400 0.35400 0.35400 0.35400

Eigenvalues --- 0.35405 0.35405 0.35405 0.35406 0.35415

Eigenvalues --- 0.35452 0.35452 0.35452 0.35461 0.35461

Eigenvalues --- 0.35461 0.35468 0.35568 0.36108 0.36108

Eigenvalues --- 0.36108 0.36179 0.36232 0.36232 0.36232

Eigenvalues --- 0.36299 0.36742 0.36873 0.37380 0.37408

Eigenvalues --- 0.38284 0.39523 0.41095 0.41997 0.41997

Eigenvalues --- 0.41997 0.42160 0.42160 0.42160 0.42178

Eigenvalues --- 0.42653 0.43248 0.43482 0.44372 0.44413

Eigenvalues --- 0.44836 0.45310 0.45484 0.45537 0.45563

Eigenvalues --- 0.45632 0.45856 0.45856 0.45856 0.45924

Eigenvalues --- 0.46150 0.46150 0.46150 0.46271 0.46380

Eigenvalues --- 0.46645 0.46645 0.46645 0.46649 0.46834

Eigenvalues --- 0.46834 0.46834 0.47401 0.47711 0.48570

Eigenvalues --- 0.48597 0.48626 0.49734 0.49854 0.50644

Eigenvalues --- 0.52869 0.53076 0.56338

En-DIIS/RFO-DIIS IScMMF= 0 using points: 10 9 8 7 6

RFO step: Lambda=-8.58908121D-08.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 8.60D-05 SmlDif= 1.00D-05

RMS Error= 0.2541727950D-04 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 0.85412 0.24479 -0.07504 -0.05663 0.03276

Iteration 1 RMS(Cart)= 0.00034531 RMS(Int)= 0.00000025

Iteration 2 RMS(Cart)= 0.00000007 RMS(Int)= 0.00000024

ITry= 1 IFail=0 DXMaxC= 1.39D-03 DCOld= 1.00D+10 DXMaxT= 7.98D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 6.26D-09 for atom 69.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.69518 -0.00003 -0.00004 -0.00003 -0.00008 2.69511

R2 2.59639 0.00004 0.00005 0.00002 0.00007 2.59646

R3 2.03620 0.00000 -0.00001 0.00001 -0.00000 2.03620

R4 2.59005 0.00001 -0.00002 0.00002 0.00000 2.59005

R5 2.67148 0.00001 0.00008 -0.00002 0.00005 2.67153

R6 2.59005 0.00001 -0.00002 0.00002 0.00000 2.59005

R7 1.91031 -0.00001 0.00003 -0.00003 -0.00000 1.91030

R8 2.69518 -0.00003 -0.00004 -0.00003 -0.00008 2.69511

R9 2.67148 0.00001 0.00008 -0.00002 0.00005 2.67153

R10 2.03620 0.00000 -0.00001 0.00001 -0.00000 2.03620

R11 2.66610 0.00002 -0.00001 0.00005 0.00004 2.66614

R12 2.79804 0.00000 -0.00002 0.00001 -0.00000 2.79804

R13 2.58128 0.00004 -0.00000 0.00007 0.00006 2.58134

R14 2.74989 -0.00001 -0.00002 -0.00001 -0.00003 2.74985

R15 2.58128 0.00004 -0.00000 0.00007 0.00006 2.58134

R16 2.74989 -0.00001 -0.00002 -0.00001 -0.00003 2.74985

R17 2.66610 0.00002 -0.00001 0.00005 0.00004 2.66614

R18 2.56229 -0.00001 -0.00000 -0.00001 -0.00001 2.56228

R19 2.03824 -0.00000 -0.00001 -0.00000 -0.00001 2.03823

R20 2.03824 -0.00000 -0.00001 -0.00000 -0.00001 2.03823

R21 2.66610 0.00002 -0.00001 0.00005 0.00004 2.66614

R22 2.79804 0.00000 -0.00002 0.00001 -0.00000 2.79804

R23 2.74989 -0.00001 -0.00002 -0.00001 -0.00003 2.74985

R24 2.58128 0.00004 -0.00000 0.00007 0.00006 2.58134

R25 2.56229 -0.00001 -0.00000 -0.00001 -0.00001 2.56228

R26 2.03824 -0.00000 -0.00001 -0.00000 -0.00001 2.03823

R27 2.74989 -0.00001 -0.00002 -0.00001 -0.00003 2.74985

R28 2.03824 -0.00000 -0.00001 -0.00000 -0.00001 2.03823

R29 2.58128 0.00004 -0.00000 0.00007 0.00006 2.58134

R30 2.66610 0.00002 -0.00001 0.00005 0.00004 2.66614

R31 2.67148 0.00001 0.00008 -0.00002 0.00005 2.67153

R32 2.79804 0.00000 -0.00002 0.00001 -0.00000 2.79804

R33 2.69518 -0.00003 -0.00004 -0.00003 -0.00008 2.69511

R34 2.59005 0.00001 -0.00002 0.00002 0.00000 2.59005

R35 2.59639 0.00004 0.00005 0.00002 0.00007 2.59646

R36 2.03620 0.00000 -0.00001 0.00001 -0.00000 2.03620

R37 2.69518 -0.00003 -0.00004 -0.00003 -0.00008 2.69511

R38 2.03620 0.00000 -0.00001 0.00001 -0.00000 2.03620

R39 2.59005 0.00001 -0.00002 0.00002 0.00000 2.59005

R40 2.67148 0.00001 0.00008 -0.00002 0.00005 2.67153

R41 1.91031 -0.00001 0.00003 -0.00003 -0.00000 1.91030

R42 2.79804 0.00000 -0.00002 0.00001 -0.00000 2.79804

R43 2.65120 -0.00000 0.00002 -0.00003 -0.00001 2.65119

R44 2.65111 0.00002 0.00002 0.00001 0.00002 2.65114

R45 2.62815 0.00000 0.00000 0.00000 0.00000 2.62816

R46 2.04814 -0.00000 -0.00001 0.00000 -0.00001 2.04814

R47 2.63516 0.00000 -0.00001 0.00001 0.00000 2.63516

R48 2.04946 -0.00000 0.00000 -0.00000 -0.00000 2.04946

R49 2.63560 -0.00000 -0.00000 -0.00000 -0.00000 2.63559

R50 2.04976 0.00000 -0.00000 0.00000 0.00000 2.04976

R51 2.62761 0.00000 0.00000 -0.00000 0.00000 2.62761

R52 2.04948 -0.00000 0.00000 -0.00000 -0.00000 2.04947

R53 2.04790 -0.00001 -0.00001 -0.00001 -0.00002 2.04788

R54 2.63516 0.00000 -0.00001 0.00001 0.00000 2.63516

R55 2.63560 -0.00000 -0.00000 -0.00000 -0.00000 2.63559

R56 2.04976 0.00000 -0.00000 0.00000 0.00000 2.04976

R57 2.62815 0.00000 0.00000 0.00000 0.00000 2.62816

R58 2.04946 -0.00000 0.00000 -0.00000 -0.00000 2.04946

R59 2.65120 -0.00000 0.00002 -0.00003 -0.00001 2.65119

R60 2.04814 -0.00000 -0.00001 0.00000 -0.00001 2.04814

R61 2.65111 0.00002 0.00002 0.00001 0.00002 2.65114

R62 2.62761 0.00000 0.00000 -0.00000 0.00000 2.62761

R63 2.04790 -0.00001 -0.00001 -0.00001 -0.00002 2.04788

R64 2.04948 -0.00000 0.00000 -0.00000 -0.00000 2.04947

R65 2.65111 0.00002 0.00002 0.00001 0.00002 2.65114

R66 2.65120 -0.00000 0.00002 -0.00003 -0.00001 2.65119

R67 2.62761 0.00000 0.00000 -0.00000 0.00000 2.62761

R68 2.04790 -0.00001 -0.00001 -0.00001 -0.00002 2.04788

R69 2.63560 -0.00000 -0.00000 -0.00000 -0.00000 2.63559

R70 2.04948 -0.00000 0.00000 -0.00000 -0.00000 2.04947

R71 2.63516 0.00000 -0.00001 0.00001 0.00000 2.63516

R72 2.04976 0.00000 -0.00000 0.00000 0.00000 2.04976

R73 2.62815 0.00000 0.00000 0.00000 0.00000 2.62816

R74 2.04946 -0.00000 0.00000 -0.00000 -0.00000 2.04946

R75 2.04814 -0.00000 -0.00001 0.00000 -0.00001 2.04814

R76 2.65111 0.00002 0.00002 0.00001 0.00002 2.65114

R77 2.65120 -0.00000 0.00002 -0.00003 -0.00001 2.65119

R78 2.62761 0.00000 0.00000 -0.00000 0.00000 2.62761

R79 2.04790 -0.00001 -0.00001 -0.00001 -0.00002 2.04788

R80 2.63560 -0.00000 -0.00000 -0.00000 -0.00000 2.63559

R81 2.04948 -0.00000 0.00000 -0.00000 -0.00000 2.04947

R82 2.63516 0.00000 -0.00001 0.00001 0.00000 2.63516

R83 2.04976 0.00000 -0.00000 0.00000 0.00000 2.04976

R84 2.62815 0.00000 0.00000 0.00000 0.00000 2.62816

R85 2.04946 -0.00000 0.00000 -0.00000 -0.00000 2.04946

R86 2.04814 -0.00000 -0.00001 0.00000 -0.00001 2.04814

A1 1.88299 -0.00000 -0.00002 0.00000 -0.00002 1.88297

A2 2.18283 0.00001 0.00003 0.00001 0.00004 2.18287

A3 2.21703 -0.00001 -0.00001 -0.00001 -0.00002 2.21701

A4 1.86614 0.00001 0.00004 0.00002 0.00006 1.86620

A5 2.21498 -0.00002 -0.00006 -0.00004 -0.00010 2.21488

A6 2.20190 0.00001 0.00001 0.00002 0.00003 2.20193

A7 1.92575 -0.00002 -0.00004 -0.00002 -0.00006 1.92570

A8 2.17869 0.00001 0.00002 0.00001 0.00002 2.17871

A9 2.17869 0.00001 0.00002 0.00001 0.00002 2.17871

A10 1.86614 0.00001 0.00004 0.00002 0.00006 1.86620

A11 2.20190 0.00001 0.00001 0.00002 0.00003 2.20193

A12 2.21498 -0.00002 -0.00006 -0.00004 -0.00010 2.21488

A13 1.88299 -0.00000 -0.00002 0.00000 -0.00002 1.88297

A14 2.21703 -0.00001 -0.00001 -0.00001 -0.00002 2.21701

A15 2.18283 0.00001 0.00003 0.00001 0.00004 2.18287

A16 2.18115 -0.00001 -0.00002 -0.00001 -0.00002 2.18113

A17 2.03763 -0.00002 -0.00001 -0.00002 -0.00004 2.03760

A18 2.06439 0.00003 0.00003 0.00003 0.00006 2.06445

A19 2.18345 -0.00001 -0.00005 0.00002 -0.00003 2.18342

A20 2.16498 0.00002 0.00003 0.00004 0.00007 2.16505

A21 1.93451 -0.00001 0.00002 -0.00005 -0.00004 1.93447

A22 1.84219 -0.00000 -0.00003 0.00004 0.00002 1.84220

A23 1.93451 -0.00001 0.00002 -0.00005 -0.00004 1.93447

A24 2.18345 -0.00001 -0.00005 0.00002 -0.00003 2.18342

A25 2.16498 0.00002 0.00003 0.00004 0.00007 2.16505

A26 1.85621 0.00001 -0.00001 0.00004 0.00003 1.85624

A27 2.19978 -0.00000 0.00002 -0.00003 -0.00001 2.19977

A28 2.22676 -0.00001 -0.00002 -0.00000 -0.00002 2.22674

A29 1.85621 0.00001 -0.00001 0.00004 0.00003 1.85624

A30 2.19978 -0.00000 0.00002 -0.00003 -0.00001 2.19977

A31 2.22676 -0.00001 -0.00002 -0.00000 -0.00002 2.22674

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D3 -3.09361 -0.00001 -0.00003 -0.00029 -0.00032 -3.09393

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D11 3.08655 0.00001 0.00018 0.00004 0.00022 3.08677

D12 -0.06573 -0.00001 0.00015 -0.00084 -0.00069 -0.06642

D13 -2.97731 -0.00001 0.00010 -0.00046 -0.00036 -2.97767

D14 0.15917 -0.00000 0.00018 -0.00034 -0.00016 0.15901

D15 0.18645 0.00000 0.00020 -0.00020 0.00001 0.18646

D16 -2.96025 0.00001 0.00028 -0.00007 0.00021 -2.96004

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D32 -0.16159 -0.00001 -0.00018 -0.00009 -0.00028 -0.16187

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D173 3.13246 0.00000 -0.00002 0.00008 0.00005 3.13251

D174 0.01971 0.00000 0.00005 -0.00001 0.00004 0.01975

D175 -0.00959 -0.00000 -0.00004 -0.00015 -0.00018 -0.00977

D176 -3.12235 -0.00000 0.00003 -0.00023 -0.00020 -3.12254

D177 0.01827 -0.00000 0.00004 -0.00007 -0.00003 0.01824

D178 -3.12328 -0.00000 0.00007 -0.00011 -0.00004 -3.12332

D179 3.13180 -0.00000 -0.00003 0.00004 0.00002 3.13182

D180 -0.00975 -0.00000 -0.00000 0.00001 0.00000 -0.00974

D181 -0.00920 -0.00000 -0.00003 -0.00005 -0.00008 -0.00928

D182 3.13242 0.00000 -0.00003 0.00004 0.00002 3.13243

D183 3.13235 -0.00000 -0.00005 -0.00002 -0.00006 3.13229

D184 -0.00922 0.00000 -0.00005 0.00008 0.00003 -0.00919

D185 -0.00926 0.00000 -0.00002 0.00007 0.00005 -0.00921

D186 3.13230 0.00000 -0.00004 0.00012 0.00008 3.13239

D187 3.13231 -0.00000 -0.00002 -0.00002 -0.00004 3.13227

D188 -0.00931 -0.00000 -0.00004 0.00003 -0.00001 -0.00932

D189 0.01867 0.00000 0.00005 0.00003 0.00008 0.01875

D190 3.13128 0.00000 -0.00002 0.00011 0.00009 3.13138

D191 -3.12289 0.00000 0.00007 -0.00002 0.00005 -3.12285

D192 -0.01028 0.00000 -0.00000 0.00006 0.00006 -0.01022

D193 -3.13228 0.00000 0.00003 0.00005 0.00008 -3.13220

D194 -0.01858 0.00000 -0.00004 0.00017 0.00012 -0.01846

D195 0.00886 -0.00000 0.00001 -0.00017 -0.00016 0.00870

D196 3.12255 -0.00000 -0.00006 -0.00006 -0.00011 3.12244

D197 -3.13246 -0.00000 0.00002 -0.00008 -0.00005 -3.13251

D198 -0.01971 -0.00000 -0.00005 0.00001 -0.00004 -0.01975

D199 0.00959 0.00000 0.00004 0.00015 0.00018 0.00977

D200 3.12235 0.00000 -0.00003 0.00023 0.00020 3.12254

D201 -0.01827 0.00000 -0.00004 0.00007 0.00003 -0.01824

D202 3.12328 0.00000 -0.00007 0.00011 0.00004 3.12332

D203 -3.13180 0.00000 0.00003 -0.00004 -0.00002 -3.13182

D204 0.00975 0.00000 0.00000 -0.00001 -0.00000 0.00974

D205 0.00920 0.00000 0.00003 0.00005 0.00008 0.00928

D206 -3.13242 -0.00000 0.00003 -0.00004 -0.00002 -3.13243

D207 -3.13235 0.00000 0.00005 0.00002 0.00006 -3.13229

D208 0.00922 -0.00000 0.00005 -0.00008 -0.00003 0.00919

D209 0.00926 -0.00000 0.00002 -0.00007 -0.00005 0.00921

D210 -3.13230 -0.00000 0.00004 -0.00012 -0.00008 -3.13239

D211 -3.13231 0.00000 0.00002 0.00002 0.00004 -3.13227

D212 0.00931 0.00000 0.00004 -0.00003 0.00001 0.00932

D213 -0.01867 -0.00000 -0.00005 -0.00003 -0.00008 -0.01875

D214 -3.13128 -0.00000 0.00002 -0.00011 -0.00009 -3.13138

D215 3.12289 -0.00000 -0.00007 0.00002 -0.00005 3.12285

D216 0.01028 -0.00000 0.00000 -0.00006 -0.00006 0.01022

Item Value Threshold Converged?

Maximum Force 0.000038 0.000450 YES

RMS Force 0.000009 0.000300 YES

Maximum Displacement 0.001388 0.001800 YES

RMS Displacement 0.000345 0.001200 YES

Predicted change in Energy=-1.421300D-07

Optimization completed.

-- Stationary point found.

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! Optimized Parameters !

! (Angstroms and Degrees) !

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! Name Definition Value Derivative Info. !

--------------------------------------------------------------------------------

! R1 R(1,2) 1.4262 -DE/DX = 0.0 !

! R2 R(1,5) 1.374 -DE/DX = 0.0 !

! R3 R(1,49) 1.0775 -DE/DX = 0.0 !

! R4 R(2,3) 1.3706 -DE/DX = 0.0 !

! R5 R(2,12) 1.4137 -DE/DX = 0.0 !

! R6 R(3,4) 1.3706 -DE/DX = 0.0 !

! R7 R(3,77) 1.0109 -DE/DX = 0.0 !

! R8 R(4,5) 1.4262 -DE/DX = 0.0 !

! R9 R(4,6) 1.4137 -DE/DX = 0.0 !

! R10 R(5,50) 1.0775 -DE/DX = 0.0 !

! R11 R(6,7) 1.4108 -DE/DX = 0.0 !

! R12 R(6,25) 1.4807 -DE/DX = 0.0 !

! R13 R(7,8) 1.366 -DE/DX = 0.0 !

! R14 R(7,11) 1.4552 -DE/DX = 0.0 !

! R15 R(8,9) 1.366 -DE/DX = 0.0 !

! R16 R(9,10) 1.4552 -DE/DX = 0.0 !

! R17 R(9,24) 1.4108 -DE/DX = 0.0 !

! R18 R(10,11) 1.3559 -DE/DX = 0.0 !

! R19 R(10,51) 1.0786 -DE/DX = 0.0 !

! R20 R(11,52) 1.0786 -DE/DX = 0.0 !

! R21 R(12,13) 1.4108 -DE/DX = 0.0 !

! R22 R(12,34) 1.4807 -DE/DX = 0.0 !

! R23 R(13,14) 1.4552 -DE/DX = 0.0 !

! R24 R(13,17) 1.366 -DE/DX = 0.0 !

! R25 R(14,15) 1.3559 -DE/DX = 0.0 !

! R26 R(14,53) 1.0786 -DE/DX = 0.0 !

! R27 R(15,16) 1.4552 -DE/DX = 0.0 !

! R28 R(15,54) 1.0786 -DE/DX = 0.0 !

! R29 R(16,17) 1.366 -DE/DX = 0.0 !

! R30 R(16,18) 1.4108 -DE/DX = 0.0 !

! R31 R(18,19) 1.4137 -DE/DX = 0.0 !

! R32 R(18,43) 1.4807 -DE/DX = 0.0 !

! R33 R(19,20) 1.4262 -DE/DX = 0.0 !

! R34 R(19,23) 1.3706 -DE/DX = 0.0 !

! R35 R(20,21) 1.374 -DE/DX = 0.0 !

! R36 R(20,55) 1.0775 -DE/DX = 0.0 !

! R37 R(21,22) 1.4262 -DE/DX = 0.0 !

! R38 R(21,56) 1.0775 -DE/DX = 0.0 !

! R39 R(22,23) 1.3706 -DE/DX = 0.0 !

! R40 R(22,24) 1.4137 -DE/DX = 0.0 !

! R41 R(23,78) 1.0109 -DE/DX = 0.0 !

! R42 R(24,37) 1.4807 -DE/DX = 0.0 !

! R43 R(25,26) 1.403 -DE/DX = 0.0 !

! R44 R(25,30) 1.4029 -DE/DX = 0.0 !

! R45 R(26,27) 1.3908 -DE/DX = 0.0 !

! R46 R(26,57) 1.0838 -DE/DX = 0.0 !

! R47 R(27,28) 1.3945 -DE/DX = 0.0 !

! R48 R(27,58) 1.0845 -DE/DX = 0.0 !

! R49 R(28,29) 1.3947 -DE/DX = 0.0 !

! R50 R(28,59) 1.0847 -DE/DX = 0.0 !

! R51 R(29,30) 1.3905 -DE/DX = 0.0 !

! R52 R(29,60) 1.0845 -DE/DX = 0.0 !

! R53 R(30,61) 1.0837 -DE/DX = 0.0 !

! R54 R(31,32) 1.3945 -DE/DX = 0.0 !

! R55 R(31,36) 1.3947 -DE/DX = 0.0 !

! R56 R(31,62) 1.0847 -DE/DX = 0.0 !

! R57 R(32,33) 1.3908 -DE/DX = 0.0 !

! R58 R(32,63) 1.0845 -DE/DX = 0.0 !

! R59 R(33,34) 1.403 -DE/DX = 0.0 !

! R60 R(33,64) 1.0838 -DE/DX = 0.0 !

! R61 R(34,35) 1.4029 -DE/DX = 0.0 !

! R62 R(35,36) 1.3905 -DE/DX = 0.0 !

! R63 R(35,65) 1.0837 -DE/DX = 0.0 !

! R64 R(36,66) 1.0845 -DE/DX = 0.0 !

! R65 R(37,38) 1.4029 -DE/DX = 0.0 !

! R66 R(37,42) 1.403 -DE/DX = 0.0 !

! R67 R(38,39) 1.3905 -DE/DX = 0.0 !

! R68 R(38,67) 1.0837 -DE/DX = 0.0 !

! R69 R(39,40) 1.3947 -DE/DX = 0.0 !

! R70 R(39,68) 1.0845 -DE/DX = 0.0 !

! R71 R(40,41) 1.3945 -DE/DX = 0.0 !

! R72 R(40,69) 1.0847 -DE/DX = 0.0 !

! R73 R(41,42) 1.3908 -DE/DX = 0.0 !

! R74 R(41,70) 1.0845 -DE/DX = 0.0 !

! R75 R(42,71) 1.0838 -DE/DX = 0.0 !

! R76 R(43,44) 1.4029 -DE/DX = 0.0 !

! R77 R(43,48) 1.403 -DE/DX = 0.0 !

! R78 R(44,45) 1.3905 -DE/DX = 0.0 !

! R79 R(44,72) 1.0837 -DE/DX = 0.0 !

! R80 R(45,46) 1.3947 -DE/DX = 0.0 !

! R81 R(45,73) 1.0845 -DE/DX = 0.0 !

! R82 R(46,47) 1.3945 -DE/DX = 0.0 !

! R83 R(46,74) 1.0847 -DE/DX = 0.0 !

! R84 R(47,48) 1.3908 -DE/DX = 0.0 !

! R85 R(47,75) 1.0845 -DE/DX = 0.0 !

! R86 R(48,76) 1.0838 -DE/DX = 0.0 !

! A1 A(2,1,5) 107.8874 -DE/DX = 0.0 !

! A2 A(2,1,49) 125.0671 -DE/DX = 0.0 !

! A3 A(5,1,49) 127.0265 -DE/DX = 0.0 !

! A4 A(1,2,3) 106.9219 -DE/DX = 0.0 !

! A5 A(1,2,12) 126.909 -DE/DX = 0.0 !

! A6 A(3,2,12) 126.1596 -DE/DX = 0.0 !

! A7 A(2,3,4) 110.3375 -DE/DX = 0.0 !

! A8 A(2,3,77) 124.8297 -DE/DX = 0.0 !

! A9 A(4,3,77) 124.8297 -DE/DX = 0.0 !

! A10 A(3,4,5) 106.9219 -DE/DX = 0.0 !

! A11 A(3,4,6) 126.1596 -DE/DX = 0.0 !

! A12 A(5,4,6) 126.909 -DE/DX = 0.0 !

! A13 A(1,5,4) 107.8874 -DE/DX = 0.0 !

! A14 A(1,5,50) 127.0265 -DE/DX = 0.0 !

! A15 A(4,5,50) 125.0671 -DE/DX = 0.0 !

! A16 A(4,6,7) 124.9707 -DE/DX = 0.0 !

! A17 A(4,6,25) 116.7478 -DE/DX = 0.0 !

! A18 A(7,6,25) 118.2809 -DE/DX = 0.0 !

! A19 A(6,7,8) 125.1024 -DE/DX = 0.0 !

! A20 A(6,7,11) 124.0442 -DE/DX = 0.0 !

! A21 A(8,7,11) 110.8391 -DE/DX = 0.0 !

! A22 A(7,8,9) 105.5494 -DE/DX = 0.0 !

! A23 A(8,9,10) 110.8391 -DE/DX = 0.0 !

! A24 A(8,9,24) 125.1024 -DE/DX = 0.0 !

! A25 A(10,9,24) 124.0442 -DE/DX = 0.0 !

! A26 A(9,10,11) 106.3528 -DE/DX = 0.0 !

! A27 A(9,10,51) 126.0383 -DE/DX = 0.0 !

! A28 A(11,10,51) 127.5841 -DE/DX = 0.0 !

! A29 A(7,11,10) 106.3528 -DE/DX = 0.0 !

! A30 A(7,11,52) 126.0383 -DE/DX = 0.0 !

! A31 A(10,11,52) 127.5841 -DE/DX = 0.0 !

! A32 A(2,12,13) 124.9707 -DE/DX = 0.0 !

! A33 A(2,12,34) 116.7478 -DE/DX = 0.0 !

! A34 A(13,12,34) 118.2809 -DE/DX = 0.0 !

! A35 A(12,13,14) 124.0442 -DE/DX = 0.0 !

! A36 A(12,13,17) 125.1024 -DE/DX = 0.0 !

! A37 A(14,13,17) 110.8391 -DE/DX = 0.0 !

! A38 A(13,14,15) 106.3528 -DE/DX = 0.0 !

! A39 A(13,14,53) 126.0383 -DE/DX = 0.0 !

! A40 A(15,14,53) 127.5841 -DE/DX = 0.0 !

! A41 A(14,15,16) 106.3528 -DE/DX = 0.0 !

! A42 A(14,15,54) 127.5841 -DE/DX = 0.0 !

! A43 A(16,15,54) 126.0383 -DE/DX = 0.0 !

! A44 A(15,16,17) 110.8391 -DE/DX = 0.0 !

! A45 A(15,16,18) 124.0442 -DE/DX = 0.0 !

! A46 A(17,16,18) 125.1024 -DE/DX = 0.0 !

! A47 A(13,17,16) 105.5494 -DE/DX = 0.0 !

! A48 A(16,18,19) 124.9707 -DE/DX = 0.0 !

! A49 A(16,18,43) 118.2809 -DE/DX = 0.0 !

! A50 A(19,18,43) 116.7478 -DE/DX = 0.0 !

! A51 A(18,19,20) 126.909 -DE/DX = 0.0 !

! A52 A(18,19,23) 126.1596 -DE/DX = 0.0 !

! A53 A(20,19,23) 106.9219 -DE/DX = 0.0 !

! A54 A(19,20,21) 107.8874 -DE/DX = 0.0 !

! A55 A(19,20,55) 125.0671 -DE/DX = 0.0 !

! A56 A(21,20,55) 127.0265 -DE/DX = 0.0 !

! A57 A(20,21,22) 107.8874 -DE/DX = 0.0 !

! A58 A(20,21,56) 127.0265 -DE/DX = 0.0 !

! A59 A(22,21,56) 125.0671 -DE/DX = 0.0 !

! A60 A(21,22,23) 106.9219 -DE/DX = 0.0 !

! A61 A(21,22,24) 126.909 -DE/DX = 0.0 !

! A62 A(23,22,24) 126.1596 -DE/DX = 0.0 !

! A63 A(19,23,22) 110.3375 -DE/DX = 0.0 !

! A64 A(19,23,78) 124.8297 -DE/DX = 0.0 !

! A65 A(22,23,78) 124.8297 -DE/DX = 0.0 !

! A66 A(9,24,22) 124.9707 -DE/DX = 0.0 !

! A67 A(9,24,37) 118.2809 -DE/DX = 0.0 !

! A68 A(22,24,37) 116.7478 -DE/DX = 0.0 !

! A69 A(6,25,26) 120.6098 -DE/DX = 0.0 !

! A70 A(6,25,30) 120.2601 -DE/DX = 0.0 !

! A71 A(26,25,30) 119.1301 -DE/DX = 0.0 !

! A72 A(25,26,27) 120.3231 -DE/DX = 0.0 !

! A73 A(25,26,57) 119.5937 -DE/DX = 0.0 !

! A74 A(27,26,57) 120.0625 -DE/DX = 0.0 !

! A75 A(26,27,28) 120.1543 -DE/DX = 0.0 !

! A76 A(26,27,58) 119.6758 -DE/DX = 0.0 !

! A77 A(28,27,58) 120.1699 -DE/DX = 0.0 !

! A78 A(27,28,29) 119.8931 -DE/DX = 0.0 !

! A79 A(27,28,59) 120.0544 -DE/DX = 0.0 !

! A80 A(29,28,59) 120.0524 -DE/DX = 0.0 !

! A81 A(28,29,30) 120.1541 -DE/DX = 0.0 !

! A82 A(28,29,60) 120.1665 -DE/DX = 0.0 !

! A83 A(30,29,60) 119.6794 -DE/DX = 0.0 !

! A84 A(25,30,29) 120.3326 -DE/DX = 0.0 !

! A85 A(25,30,61) 119.5386 -DE/DX = 0.0 !

! A86 A(29,30,61) 120.1095 -DE/DX = 0.0 !

! A87 A(32,31,36) 119.8931 -DE/DX = 0.0 !

! A88 A(32,31,62) 120.0544 -DE/DX = 0.0 !

! A89 A(36,31,62) 120.0524 -DE/DX = 0.0 !

! A90 A(31,32,33) 120.1543 -DE/DX = 0.0 !

! A91 A(31,32,63) 120.1699 -DE/DX = 0.0 !

! A92 A(33,32,63) 119.6758 -DE/DX = 0.0 !

! A93 A(32,33,34) 120.3231 -DE/DX = 0.0 !

! A94 A(32,33,64) 120.0625 -DE/DX = 0.0 !

! A95 A(34,33,64) 119.5937 -DE/DX = 0.0 !

! A96 A(12,34,33) 120.6098 -DE/DX = 0.0 !

! A97 A(12,34,35) 120.2601 -DE/DX = 0.0 !

! A98 A(33,34,35) 119.1301 -DE/DX = 0.0 !

! A99 A(34,35,36) 120.3326 -DE/DX = 0.0 !

! A100 A(34,35,65) 119.5386 -DE/DX = 0.0 !

! A101 A(36,35,65) 120.1095 -DE/DX = 0.0 !

! A102 A(31,36,35) 120.1541 -DE/DX = 0.0 !

! A103 A(31,36,66) 120.1665 -DE/DX = 0.0 !

! A104 A(35,36,66) 119.6794 -DE/DX = 0.0 !

! A105 A(24,37,38) 120.2601 -DE/DX = 0.0 !

! A106 A(24,37,42) 120.6098 -DE/DX = 0.0 !

! A107 A(38,37,42) 119.1301 -DE/DX = 0.0 !

! A108 A(37,38,39) 120.3326 -DE/DX = 0.0 !

! A109 A(37,38,67) 119.5386 -DE/DX = 0.0 !

! A110 A(39,38,67) 120.1095 -DE/DX = 0.0 !

! A111 A(38,39,40) 120.1541 -DE/DX = 0.0 !

! A112 A(38,39,68) 119.6794 -DE/DX = 0.0 !

! A113 A(40,39,68) 120.1665 -DE/DX = 0.0 !

! A114 A(39,40,41) 119.8931 -DE/DX = 0.0 !

! A115 A(39,40,69) 120.0524 -DE/DX = 0.0 !

! A116 A(41,40,69) 120.0544 -DE/DX = 0.0 !

! A117 A(40,41,42) 120.1543 -DE/DX = 0.0 !

! A118 A(40,41,70) 120.1699 -DE/DX = 0.0 !

! A119 A(42,41,70) 119.6758 -DE/DX = 0.0 !

! A120 A(37,42,41) 120.3231 -DE/DX = 0.0 !

! A121 A(37,42,71) 119.5937 -DE/DX = 0.0 !

! A122 A(41,42,71) 120.0625 -DE/DX = 0.0 !

! A123 A(18,43,44) 120.2601 -DE/DX = 0.0 !

! A124 A(18,43,48) 120.6098 -DE/DX = 0.0 !

! A125 A(44,43,48) 119.1301 -DE/DX = 0.0 !

! A126 A(43,44,45) 120.3326 -DE/DX = 0.0 !

! A127 A(43,44,72) 119.5386 -DE/DX = 0.0 !

! A128 A(45,44,72) 120.1095 -DE/DX = 0.0 !

! A129 A(44,45,46) 120.1541 -DE/DX = 0.0 !

! A130 A(44,45,73) 119.6794 -DE/DX = 0.0 !

! A131 A(46,45,73) 120.1665 -DE/DX = 0.0 !

! A132 A(45,46,47) 119.8931 -DE/DX = 0.0 !

! A133 A(45,46,74) 120.0524 -DE/DX = 0.0 !

! A134 A(47,46,74) 120.0544 -DE/DX = 0.0 !

! A135 A(46,47,48) 120.1543 -DE/DX = 0.0 !

! A136 A(46,47,75) 120.1699 -DE/DX = 0.0 !

! A137 A(48,47,75) 119.6758 -DE/DX = 0.0 !

! A138 A(43,48,47) 120.3231 -DE/DX = 0.0 !

! A139 A(43,48,76) 119.5937 -DE/DX = 0.0 !

! A140 A(47,48,76) 120.0625 -DE/DX = 0.0 !

! D1 D(5,1,2,3) 1.2552 -DE/DX = 0.0 !

! D2 D(5,1,2,12) -177.6727 -DE/DX = 0.0 !

! D3 D(49,1,2,3) -177.2509 -DE/DX = 0.0 !

! D4 D(49,1,2,12) 3.8212 -DE/DX = 0.0 !

! D5 D(2,1,5,4) 0.0 -DE/DX = 0.0 !

! D6 D(2,1,5,50) -178.4685 -DE/DX = 0.0 !

! D7 D(49,1,5,4) 178.4685 -DE/DX = 0.0 !

! D8 D(49,1,5,50) 0.0 -DE/DX = 0.0 !

! D9 D(1,2,3,4) -2.0917 -DE/DX = 0.0 !

! D10 D(1,2,3,77) 177.2955 -DE/DX = 0.0 !

! D11 D(12,2,3,4) 176.8465 -DE/DX = 0.0 !

! D12 D(12,2,3,77) -3.7663 -DE/DX = 0.0 !

! D13 D(1,2,12,13) -170.5875 -DE/DX = 0.0 !

! D14 D(1,2,12,34) 9.1198 -DE/DX = 0.0 !

! D15 D(3,2,12,13) 10.6829 -DE/DX = 0.0 !

! D16 D(3,2,12,34) -169.6098 -DE/DX = 0.0 !

! D17 D(2,3,4,5) 2.0917 -DE/DX = 0.0 !

! D18 D(2,3,4,6) -176.8465 -DE/DX = 0.0 !

! D19 D(77,3,4,5) -177.2955 -DE/DX = 0.0 !

! D20 D(77,3,4,6) 3.7663 -DE/DX = 0.0 !

! D21 D(3,4,5,1) -1.2552 -DE/DX = 0.0 !

! D22 D(3,4,5,50) 177.2509 -DE/DX = 0.0 !

! D23 D(6,4,5,1) 177.6727 -DE/DX = 0.0 !

! D24 D(6,4,5,50) -3.8212 -DE/DX = 0.0 !

! D25 D(3,4,6,7) -10.6829 -DE/DX = 0.0 !

! D26 D(3,4,6,25) 169.6098 -DE/DX = 0.0 !

! D27 D(5,4,6,7) 170.5875 -DE/DX = 0.0 !

! D28 D(5,4,6,25) -9.1198 -DE/DX = 0.0 !

! D29 D(4,6,7,8) -10.4669 -DE/DX = 0.0 !

! D30 D(4,6,7,11) 171.0382 -DE/DX = 0.0 !

! D31 D(25,6,7,8) 169.2363 -DE/DX = 0.0 !

! D32 D(25,6,7,11) -9.2587 -DE/DX = 0.0 !

! D33 D(4,6,25,26) -55.5653 -DE/DX = 0.0 !

! D34 D(4,6,25,30) 124.4082 -DE/DX = 0.0 !

! D35 D(7,6,25,26) 124.7071 -DE/DX = 0.0 !

! D36 D(7,6,25,30) -55.3194 -DE/DX = 0.0 !

! D37 D(6,7,8,9) -176.1152 -DE/DX = 0.0 !

! D38 D(11,7,8,9) 2.5504 -DE/DX = 0.0 !

! D39 D(6,7,11,10) 177.0749 -DE/DX = 0.0 !

! D40 D(6,7,11,52) -4.6312 -DE/DX = 0.0 !

! D41 D(8,7,11,10) -1.6076 -DE/DX = 0.0 !

! D42 D(8,7,11,52) 176.6863 -DE/DX = 0.0 !

! D43 D(7,8,9,10) -2.5504 -DE/DX = 0.0 !

! D44 D(7,8,9,24) 176.1152 -DE/DX = 0.0 !

! D45 D(8,9,10,11) 1.6076 -DE/DX = 0.0 !

! D46 D(8,9,10,51) -176.6863 -DE/DX = 0.0 !

! D47 D(24,9,10,11) -177.0749 -DE/DX = 0.0 !

! D48 D(24,9,10,51) 4.6312 -DE/DX = 0.0 !

! D49 D(8,9,24,22) 10.4669 -DE/DX = 0.0 !

! D50 D(8,9,24,37) -169.2363 -DE/DX = 0.0 !

! D51 D(10,9,24,22) -171.0382 -DE/DX = 0.0 !

! D52 D(10,9,24,37) 9.2587 -DE/DX = 0.0 !

! D53 D(9,10,11,7) 0.0 -DE/DX = 0.0 !

! D54 D(9,10,11,52) -178.2591 -DE/DX = 0.0 !

! D55 D(51,10,11,7) 178.2591 -DE/DX = 0.0 !

! D56 D(51,10,11,52) 0.0 -DE/DX = 0.0 !

! D57 D(2,12,13,14) -171.0382 -DE/DX = 0.0 !

! D58 D(2,12,13,17) 10.4669 -DE/DX = 0.0 !

! D59 D(34,12,13,14) 9.2587 -DE/DX = 0.0 !

! D60 D(34,12,13,17) -169.2363 -DE/DX = 0.0 !

! D61 D(2,12,34,33) 55.5653 -DE/DX = 0.0 !

! D62 D(2,12,34,35) -124.4082 -DE/DX = 0.0 !

! D63 D(13,12,34,33) -124.7071 -DE/DX = 0.0 !

! D64 D(13,12,34,35) 55.3194 -DE/DX = 0.0 !

! D65 D(12,13,14,15) -177.0749 -DE/DX = 0.0 !

! D66 D(12,13,14,53) 4.6312 -DE/DX = 0.0 !

! D67 D(17,13,14,15) 1.6076 -DE/DX = 0.0 !

! D68 D(17,13,14,53) -176.6863 -DE/DX = 0.0 !

! D69 D(12,13,17,16) 176.1152 -DE/DX = 0.0 !

! D70 D(14,13,17,16) -2.5504 -DE/DX = 0.0 !

! D71 D(13,14,15,16) 0.0 -DE/DX = 0.0 !

! D72 D(13,14,15,54) -178.2591 -DE/DX = 0.0 !

! D73 D(53,14,15,16) 178.2591 -DE/DX = 0.0 !

! D74 D(53,14,15,54) 0.0 -DE/DX = 0.0 !

! D75 D(14,15,16,17) -1.6076 -DE/DX = 0.0 !

! D76 D(14,15,16,18) 177.0749 -DE/DX = 0.0 !

! D77 D(54,15,16,17) 176.6863 -DE/DX = 0.0 !

! D78 D(54,15,16,18) -4.6312 -DE/DX = 0.0 !

! D79 D(15,16,17,13) 2.5504 -DE/DX = 0.0 !

! D80 D(18,16,17,13) -176.1152 -DE/DX = 0.0 !

! D81 D(15,16,18,19) 171.0382 -DE/DX = 0.0 !

! D82 D(15,16,18,43) -9.2587 -DE/DX = 0.0 !

! D83 D(17,16,18,19) -10.4669 -DE/DX = 0.0 !

! D84 D(17,16,18,43) 169.2363 -DE/DX = 0.0 !

! D85 D(16,18,19,20) 170.5875 -DE/DX = 0.0 !

! D86 D(16,18,19,23) -10.6829 -DE/DX = 0.0 !

! D87 D(43,18,19,20) -9.1198 -DE/DX = 0.0 !

! D88 D(43,18,19,23) 169.6098 -DE/DX = 0.0 !

! D89 D(16,18,43,44) -55.3194 -DE/DX = 0.0 !

! D90 D(16,18,43,48) 124.7071 -DE/DX = 0.0 !

! D91 D(19,18,43,44) 124.4082 -DE/DX = 0.0 !

! D92 D(19,18,43,48) -55.5653 -DE/DX = 0.0 !

! D93 D(18,19,20,21) 177.6727 -DE/DX = 0.0 !

! D94 D(18,19,20,55) -3.8212 -DE/DX = 0.0 !

! D95 D(23,19,20,21) -1.2552 -DE/DX = 0.0 !

! D96 D(23,19,20,55) 177.2509 -DE/DX = 0.0 !

! D97 D(18,19,23,22) -176.8465 -DE/DX = 0.0 !

! D98 D(18,19,23,78) 3.7663 -DE/DX = 0.0 !

! D99 D(20,19,23,22) 2.0917 -DE/DX = 0.0 !

! D100 D(20,19,23,78) -177.2955 -DE/DX = 0.0 !

! D101 D(19,20,21,22) 0.0 -DE/DX = 0.0 !

! D102 D(19,20,21,56) 178.4685 -DE/DX = 0.0 !

! D103 D(55,20,21,22) -178.4685 -DE/DX = 0.0 !

! D104 D(55,20,21,56) 0.0 -DE/DX = 0.0 !

! D105 D(20,21,22,23) 1.2552 -DE/DX = 0.0 !

! D106 D(20,21,22,24) -177.6727 -DE/DX = 0.0 !

! D107 D(56,21,22,23) -177.2509 -DE/DX = 0.0 !

! D108 D(56,21,22,24) 3.8212 -DE/DX = 0.0 !

! D109 D(21,22,23,19) -2.0917 -DE/DX = 0.0 !

! D110 D(21,22,23,78) 177.2955 -DE/DX = 0.0 !

! D111 D(24,22,23,19) 176.8465 -DE/DX = 0.0 !

! D112 D(24,22,23,78) -3.7663 -DE/DX = 0.0 !

! D113 D(21,22,24,9) -170.5875 -DE/DX = 0.0 !

! D114 D(21,22,24,37) 9.1198 -DE/DX = 0.0 !

! D115 D(23,22,24,9) 10.6829 -DE/DX = 0.0 !

! D116 D(23,22,24,37) -169.6098 -DE/DX = 0.0 !

! D117 D(9,24,37,38) 55.3194 -DE/DX = 0.0 !

! D118 D(9,24,37,42) -124.7071 -DE/DX = 0.0 !

! D119 D(22,24,37,38) -124.4082 -DE/DX = 0.0 !

! D120 D(22,24,37,42) 55.5653 -DE/DX = 0.0 !

! D121 D(6,25,26,27) -179.4767 -DE/DX = 0.0 !

! D122 D(6,25,26,57) -1.1291 -DE/DX = 0.0 !

! D123 D(30,25,26,27) 0.5495 -DE/DX = 0.0 !

! D124 D(30,25,26,57) 178.8972 -DE/DX = 0.0 !

! D125 D(6,25,30,29) -179.4662 -DE/DX = 0.0 !

! D126 D(6,25,30,61) -1.0646 -DE/DX = 0.0 !

! D127 D(26,25,30,29) 0.5076 -DE/DX = 0.0 !

! D128 D(26,25,30,61) 178.9092 -DE/DX = 0.0 !

! D129 D(25,26,27,28) -1.0695 -DE/DX = 0.0 !

! D130 D(25,26,27,58) 178.9287 -DE/DX = 0.0 !

! D131 D(57,26,27,28) -179.4094 -DE/DX = 0.0 !

! D132 D(57,26,27,58) 0.5888 -DE/DX = 0.0 !

! D133 D(26,27,28,29) 0.5303 -DE/DX = 0.0 !

! D134 D(26,27,28,59) -179.4683 -DE/DX = 0.0 !

! D135 D(58,27,28,29) -179.4678 -DE/DX = 0.0 !

! D136 D(58,27,28,59) 0.5336 -DE/DX = 0.0 !

! D137 D(27,28,29,30) 0.5271 -DE/DX = 0.0 !

! D138 D(27,28,29,60) -179.4706 -DE/DX = 0.0 !

! D139 D(59,28,29,30) -179.4743 -DE/DX = 0.0 !

! D140 D(59,28,29,60) 0.528 -DE/DX = 0.0 !

! D141 D(28,29,30,25) -1.0467 -DE/DX = 0.0 !

! D142 D(28,29,30,61) -179.4392 -DE/DX = 0.0 !

! D143 D(60,29,30,25) 178.951 -DE/DX = 0.0 !

! D144 D(60,29,30,61) 0.5585 -DE/DX = 0.0 !

! D145 D(36,31,32,33) -0.5303 -DE/DX = 0.0 !

! D146 D(36,31,32,63) 179.4678 -DE/DX = 0.0 !

! D147 D(62,31,32,33) 179.4683 -DE/DX = 0.0 !

! D148 D(62,31,32,63) -0.5336 -DE/DX = 0.0 !

! D149 D(32,31,36,35) -0.5271 -DE/DX = 0.0 !

! D150 D(32,31,36,66) 179.4706 -DE/DX = 0.0 !

! D151 D(62,31,36,35) 179.4743 -DE/DX = 0.0 !

! D152 D(62,31,36,66) -0.528 -DE/DX = 0.0 !

! D153 D(31,32,33,34) 1.0695 -DE/DX = 0.0 !

! D154 D(31,32,33,64) 179.4094 -DE/DX = 0.0 !

! D155 D(63,32,33,34) -178.9287 -DE/DX = 0.0 !

! D156 D(63,32,33,64) -0.5888 -DE/DX = 0.0 !

! D157 D(32,33,34,12) 179.4767 -DE/DX = 0.0 !

! D158 D(32,33,34,35) -0.5495 -DE/DX = 0.0 !

! D159 D(64,33,34,12) 1.1291 -DE/DX = 0.0 !

! D160 D(64,33,34,35) -178.8972 -DE/DX = 0.0 !

! D161 D(12,34,35,36) 179.4662 -DE/DX = 0.0 !

! D162 D(12,34,35,65) 1.0646 -DE/DX = 0.0 !

! D163 D(33,34,35,36) -0.5076 -DE/DX = 0.0 !

! D164 D(33,34,35,65) -178.9092 -DE/DX = 0.0 !

! D165 D(34,35,36,31) 1.0467 -DE/DX = 0.0 !

! D166 D(34,35,36,66) -178.951 -DE/DX = 0.0 !

! D167 D(65,35,36,31) 179.4392 -DE/DX = 0.0 !

! D168 D(65,35,36,66) -0.5585 -DE/DX = 0.0 !

! D169 D(24,37,38,39) 179.4662 -DE/DX = 0.0 !

! D170 D(24,37,38,67) 1.0646 -DE/DX = 0.0 !

! D171 D(42,37,38,39) -0.5076 -DE/DX = 0.0 !

! D172 D(42,37,38,67) -178.9092 -DE/DX = 0.0 !

! D173 D(24,37,42,41) 179.4767 -DE/DX = 0.0 !

! D174 D(24,37,42,71) 1.1291 -DE/DX = 0.0 !

! D175 D(38,37,42,41) -0.5495 -DE/DX = 0.0 !

! D176 D(38,37,42,71) -178.8972 -DE/DX = 0.0 !

! D177 D(37,38,39,40) 1.0467 -DE/DX = 0.0 !

! D178 D(37,38,39,68) -178.951 -DE/DX = 0.0 !

! D179 D(67,38,39,40) 179.4392 -DE/DX = 0.0 !

! D180 D(67,38,39,68) -0.5585 -DE/DX = 0.0 !

! D181 D(38,39,40,41) -0.5271 -DE/DX = 0.0 !

! D182 D(38,39,40,69) 179.4743 -DE/DX = 0.0 !

! D183 D(68,39,40,41) 179.4706 -DE/DX = 0.0 !

! D184 D(68,39,40,69) -0.528 -DE/DX = 0.0 !

! D185 D(39,40,41,42) -0.5303 -DE/DX = 0.0 !

! D186 D(39,40,41,70) 179.4678 -DE/DX = 0.0 !

! D187 D(69,40,41,42) 179.4683 -DE/DX = 0.0 !

! D188 D(69,40,41,70) -0.5336 -DE/DX = 0.0 !

! D189 D(40,41,42,37) 1.0695 -DE/DX = 0.0 !

! D190 D(40,41,42,71) 179.4094 -DE/DX = 0.0 !

! D191 D(70,41,42,37) -178.9287 -DE/DX = 0.0 !

! D192 D(70,41,42,71) -0.5888 -DE/DX = 0.0 !

! D193 D(18,43,44,45) -179.4662 -DE/DX = 0.0 !

! D194 D(18,43,44,72) -1.0646 -DE/DX = 0.0 !

! D195 D(48,43,44,45) 0.5076 -DE/DX = 0.0 !

! D196 D(48,43,44,72) 178.9092 -DE/DX = 0.0 !

! D197 D(18,43,48,47) -179.4767 -DE/DX = 0.0 !

! D198 D(18,43,48,76) -1.1291 -DE/DX = 0.0 !

! D199 D(44,43,48,47) 0.5495 -DE/DX = 0.0 !

! D200 D(44,43,48,76) 178.8972 -DE/DX = 0.0 !

! D201 D(43,44,45,46) -1.0467 -DE/DX = 0.0 !

! D202 D(43,44,45,73) 178.951 -DE/DX = 0.0 !

! D203 D(72,44,45,46) -179.4392 -DE/DX = 0.0 !

! D204 D(72,44,45,73) 0.5585 -DE/DX = 0.0 !

! D205 D(44,45,46,47) 0.5271 -DE/DX = 0.0 !

! D206 D(44,45,46,74) -179.4743 -DE/DX = 0.0 !

! D207 D(73,45,46,47) -179.4706 -DE/DX = 0.0 !

! D208 D(73,45,46,74) 0.528 -DE/DX = 0.0 !

! D209 D(45,46,47,48) 0.5303 -DE/DX = 0.0 !

! D210 D(45,46,47,75) -179.4678 -DE/DX = 0.0 !

! D211 D(74,46,47,48) -179.4683 -DE/DX = 0.0 !

! D212 D(74,46,47,75) 0.5336 -DE/DX = 0.0 !

! D213 D(46,47,48,43) -1.0695 -DE/DX = 0.0 !

! D214 D(46,47,48,76) -179.4094 -DE/DX = 0.0 !

! D215 D(75,47,48,43) 178.9287 -DE/DX = 0.0 !

! D216 D(75,47,48,76) 0.5888 -DE/DX = 0.0 !

--------------------------------------------------------------------------------

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Largest change from initial coordinates is atom 58 0.162 Angstoms.

Leave Link 103 at Sun Aug 18 14:40:27 2019, MaxMem= 2013265920 cpu: 1.4

(Enter /home/kira/g09/l202.exe)

Stoichiometry C44H30N4(1+,2)

Framework group C2V[SGV(H2N2),SGV'(N2),X(C44H28)]

Deg. of freedom 59

Full point group C2V NOp 4

RotChk: IX=0 Diff= 3.49D-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 -0.686976 4.173391 0.508033

2 6 0 -1.125038 2.863317 0.153157

3 7 0 0.000000 2.100715 -0.023658

4 6 0 1.125038 2.863317 0.153157

5 6 0 0.686976 4.173391 0.508033

6 6 0 2.460643 2.430315 -0.011692

7 6 0 2.860728 1.087659 -0.178055

8 7 0 2.052997 -0.000000 -0.003699

9 6 0 2.860728 -1.087659 -0.178055

10 6 0 4.211549 -0.677953 -0.531554

11 6 0 4.211549 0.677953 -0.531554

12 6 0 -2.460643 2.430315 -0.011692

13 6 0 -2.860728 1.087659 -0.178055

14 6 0 -4.211549 0.677953 -0.531554

15 6 0 -4.211549 -0.677953 -0.531554

16 6 0 -2.860728 -1.087659 -0.178055

17 7 0 -2.052997 0.000000 -0.003699

18 6 0 -2.460643 -2.430315 -0.011692

19 6 0 -1.125038 -2.863317 0.153157

20 6 0 -0.686976 -4.173391 0.508033

21 6 0 0.686976 -4.173391 0.508033

22 6 0 1.125038 -2.863317 0.153157

23 7 0 -0.000000 -2.100715 -0.023658

24 6 0 2.460643 -2.430315 -0.011692

25 6 0 3.507012 3.477851 -0.000280

26 6 0 3.443300 4.560918 -0.889765

27 6 0 4.435149 5.535789 -0.881267

28 6 0 5.489297 5.454669 0.027976

29 6 0 5.554430 4.387244 0.923266

30 6 0 4.576893 3.398581 0.903725

31 6 0 -5.489297 5.454669 0.027976

32 6 0 -4.435149 5.535789 -0.881267

33 6 0 -3.443300 4.560918 -0.889765

34 6 0 -3.507012 3.477851 -0.000280

35 6 0 -4.576893 3.398581 0.903725

36 6 0 -5.554430 4.387244 0.923266

37 6 0 3.507012 -3.477851 -0.000280

38 6 0 4.576893 -3.398581 0.903725

39 6 0 5.554430 -4.387244 0.923266

40 6 0 5.489297 -5.454669 0.027976

41 6 0 4.435149 -5.535789 -0.881267

42 6 0 3.443300 -4.560918 -0.889765

43 6 0 -3.507012 -3.477851 -0.000280

44 6 0 -4.576893 -3.398581 0.903725

45 6 0 -5.554430 -4.387244 0.923266

46 6 0 -5.489297 -5.454669 0.027976

47 6 0 -4.435149 -5.535789 -0.881267

48 6 0 -3.443300 -4.560918 -0.889765

49 1 0 -1.335838 4.997399 0.755062

50 1 0 1.335838 4.997399 0.755062

51 1 0 5.031487 -1.335811 -0.772966

52 1 0 5.031487 1.335811 -0.772966

53 1 0 -5.031487 1.335811 -0.772966

54 1 0 -5.031487 -1.335811 -0.772966

55 1 0 -1.335838 -4.997399 0.755062

56 1 0 1.335838 -4.997399 0.755062

57 1 0 2.629785 4.620261 -1.603460

58 1 0 4.384697 6.359262 -1.585220

59 1 0 6.257368 6.220495 0.038958

60 1 0 6.367661 4.324289 1.638048

61 1 0 4.623233 2.574297 1.605736

62 1 0 -6.257368 6.220495 0.038958

63 1 0 -4.384697 6.359262 -1.585220

64 1 0 -2.629785 4.620261 -1.603460

65 1 0 -4.623233 2.574297 1.605736

66 1 0 -6.367661 4.324289 1.638048

67 1 0 4.623233 -2.574297 1.605736

68 1 0 6.367661 -4.324289 1.638048

69 1 0 6.257368 -6.220495 0.038958

70 1 0 4.384697 -6.359262 -1.585220

71 1 0 2.629785 -4.620261 -1.603460

72 1 0 -4.623233 -2.574297 1.605736

73 1 0 -6.367661 -4.324289 1.638048

74 1 0 -6.257368 -6.220495 0.038958

75 1 0 -4.384697 -6.359262 -1.585220

76 1 0 -2.629785 -4.620261 -1.603460

77 1 0 0.000000 1.113981 -0.243331

78 1 0 -0.000000 -1.113981 -0.243331

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0593157 0.0585922 0.0302906

Leave Link 202 at Sun Aug 18 14:40:27 2019, MaxMem= 2013265920 cpu: 0.1

(Enter /home/kira/g09/l601.exe)

Copying SCF densities to generalized density rwf, IOpCl= 1 IROHF=0.

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Population analysis using the SCF density.

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Orbital symmetries:

Alpha Orbitals:

Occupied (B2) (A1) (B1) (A1) (B2) (A2) (A1) (B1) (A2) (B2)

(B1) (A1) (A2) (A1) (B1) (B2) (A2) (B2) (B1) (A1)

(B2) (A1) (A2) (B1) (A2) (B1) (B2) (A1) (A2) (B2)

(B1) (A1) (A2) (B2) (B1) (A1) (A2) (B1) (B2) (A1)

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(A1)

Virtual (B1) (B2) (A2) (A1) (B2) (B1) (A2) (A2) (B2) (A1)

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The electronic state is 2-A1.

Alpha occ. eigenvalues -- -14.38079 -14.38079 -14.31812 -14.31812 -10.24413

Alpha occ. eigenvalues -- -10.24413 -10.24413 -10.24413 -10.23478 -10.23478

Alpha occ. eigenvalues -- -10.23478 -10.23477 -10.22384 -10.22384 -10.22384

Alpha occ. eigenvalues -- -10.22384 -10.20037 -10.20037 -10.20037 -10.20037

Alpha occ. eigenvalues -- -10.19322 -10.19322 -10.19260 -10.19260 -10.18512

Alpha occ. eigenvalues -- -10.18512 -10.18512 -10.18512 -10.18479 -10.18479

Alpha occ. eigenvalues -- -10.18479 -10.18479 -10.18223 -10.18223 -10.18223

Alpha occ. eigenvalues -- -10.18223 -10.17994 -10.17994 -10.17994 -10.17994

Alpha occ. eigenvalues -- -10.17986 -10.17986 -10.17986 -10.17986 -10.17897

Alpha occ. eigenvalues -- -10.17897 -10.17827 -10.17827 -1.01824 -1.01670

Alpha occ. eigenvalues -- -0.97207 -0.96916 -0.88748 -0.88081 -0.88035

Alpha occ. eigenvalues -- -0.87737 -0.84578 -0.83333 -0.82918 -0.81944

Alpha occ. eigenvalues -- -0.81317 -0.80313 -0.78147 -0.77747 -0.76194

Alpha occ. eigenvalues -- -0.75900 -0.75870 -0.75833 -0.75683 -0.75294

Alpha occ. eigenvalues -- -0.74793 -0.74179 -0.72773 -0.68973 -0.68313

Alpha occ. eigenvalues -- -0.64039 -0.62831 -0.62455 -0.62165 -0.62072

Alpha occ. eigenvalues -- -0.61667 -0.61663 -0.61647 -0.61339 -0.61014

Alpha occ. eigenvalues -- -0.60762 -0.59544 -0.58833 -0.57753 -0.56996

Alpha occ. eigenvalues -- -0.56349 -0.54505 -0.53690 -0.53326 -0.52504

Alpha occ. eigenvalues -- -0.52457 -0.51502 -0.51326 -0.50448 -0.48193

Alpha occ. eigenvalues -- -0.47943 -0.47466 -0.47175 -0.47022 -0.46928

Alpha occ. eigenvalues -- -0.46484 -0.46480 -0.46307 -0.45696 -0.45651

Alpha occ. eigenvalues -- -0.45106 -0.44698 -0.44221 -0.43865 -0.43826

Alpha occ. eigenvalues -- -0.43543 -0.43310 -0.43125 -0.43047 -0.43022

Alpha occ. eigenvalues -- -0.43008 -0.42441 -0.41969 -0.41415 -0.41201

Alpha occ. eigenvalues -- -0.41029 -0.40095 -0.39782 -0.39641 -0.39065

Alpha occ. eigenvalues -- -0.37965 -0.37928 -0.37701 -0.37534 -0.36302

Alpha occ. eigenvalues -- -0.36012 -0.35868 -0.35796 -0.35550 -0.35528

Alpha occ. eigenvalues -- -0.35523 -0.35510 -0.34234 -0.31418 -0.30975

Alpha occ. eigenvalues -- -0.30232 -0.30082 -0.28831 -0.28740 -0.28074

Alpha occ. eigenvalues -- -0.26933 -0.26927 -0.26824 -0.26668 -0.26352

Alpha occ. eigenvalues -- -0.26297 -0.26170 -0.26098 -0.26013 -0.22073

Alpha occ. eigenvalues -- -0.21691

Alpha virt. eigenvalues -- -0.12016 -0.11446 -0.06071 -0.02489 -0.02434

Alpha virt. eigenvalues -- -0.02305 -0.01954 -0.01946 -0.01795 -0.01757

Alpha virt. eigenvalues -- -0.01742 0.00818 0.03603 0.03964 0.04898

Alpha virt. eigenvalues -- 0.05321 0.05341 0.05540 0.05864 0.06648

Alpha virt. eigenvalues -- 0.07803 0.07872 0.08051 0.08737 0.09078

Alpha virt. eigenvalues -- 0.09100 0.09201 0.09306 0.09526 0.09534

Alpha virt. eigenvalues -- 0.09774 0.10000 0.10095 0.10105 0.10328

Alpha virt. eigenvalues -- 0.10756 0.12183 0.12216 0.12372 0.12404

Alpha virt. eigenvalues -- 0.12735 0.12814 0.12827 0.13404 0.13926

Alpha virt. eigenvalues -- 0.13941 0.13993 0.14164 0.14197 0.14792

Alpha virt. eigenvalues -- 0.15073 0.15160 0.15778 0.16429 0.17304

Alpha virt. eigenvalues -- 0.19872 0.20159 0.20807 0.20904 0.22361

Alpha virt. eigenvalues -- 0.22387 0.22445 0.23246 0.23809 0.24366

Alpha virt. eigenvalues -- 0.24605 0.24847 0.25091 0.25159 0.25851

Alpha virt. eigenvalues -- 0.26671 0.26841 0.27282 0.27381 0.27406

Alpha virt. eigenvalues -- 0.27546 0.27959 0.28132 0.28598 0.28761

Alpha virt. eigenvalues -- 0.28994 0.29003 0.29144 0.29736 0.30011

Alpha virt. eigenvalues -- 0.30145 0.30214 0.30445 0.30857 0.32126

Alpha virt. eigenvalues -- 0.32839 0.33265 0.33883 0.33909 0.34417

Alpha virt. eigenvalues -- 0.34592 0.34920 0.35095 0.35145 0.35690

Alpha virt. eigenvalues -- 0.35852 0.36082 0.36091 0.36533 0.36565

Alpha virt. eigenvalues -- 0.36961 0.37234 0.37425 0.37479 0.38082

Alpha virt. eigenvalues -- 0.38305 0.38615 0.39113 0.39327 0.39613

Alpha virt. eigenvalues -- 0.39671 0.40023 0.40047 0.40222 0.40369

Alpha virt. eigenvalues -- 0.40530 0.40901 0.41050 0.41052 0.41122

Alpha virt. eigenvalues -- 0.41190 0.41956 0.41989 0.42102 0.42199

Alpha virt. eigenvalues -- 0.42531 0.42856 0.42864 0.42887 0.43716

Alpha virt. eigenvalues -- 0.43827 0.44006 0.44105 0.44181 0.44421

Alpha virt. eigenvalues -- 0.44564 0.44632 0.44713 0.44800 0.44819

Alpha virt. eigenvalues -- 0.44890 0.45757 0.45991 0.46246 0.46460

Alpha virt. eigenvalues -- 0.46462 0.46503 0.47287 0.47792 0.47975

Alpha virt. eigenvalues -- 0.48215 0.48687 0.49353 0.49494 0.49656

Alpha virt. eigenvalues -- 0.50130 0.50360 0.50791 0.51682 0.51803

Alpha virt. eigenvalues -- 0.52098 0.52166 0.52936 0.53063 0.53275

Alpha virt. eigenvalues -- 0.53550 0.53743 0.54693 0.54759 0.56398

Alpha virt. eigenvalues -- 0.56630 0.56789 0.56817 0.57148 0.57254

Alpha virt. eigenvalues -- 0.57573 0.58343 0.58673 0.58739 0.59124

Alpha virt. eigenvalues -- 0.59148 0.59266 0.59358 0.59456 0.60131

Alpha virt. eigenvalues -- 0.60197 0.60212 0.60295 0.60578 0.60873

Alpha virt. eigenvalues -- 0.60900 0.60932 0.61036 0.61346 0.61436

Alpha virt. eigenvalues -- 0.61914 0.61974 0.62102 0.62786 0.62903

Alpha virt. eigenvalues -- 0.63641 0.63803 0.63933 0.64397 0.64411

Alpha virt. eigenvalues -- 0.64493 0.64663 0.64884 0.65351 0.65411

Alpha virt. eigenvalues -- 0.65512 0.66451 0.66713 0.67208 0.67732

Alpha virt. eigenvalues -- 0.67920 0.68050 0.68826 0.68908 0.68963

Alpha virt. eigenvalues -- 0.70179 0.70774 0.71140 0.71312 0.71730

Alpha virt. eigenvalues -- 0.71762 0.72391 0.72690 0.72752 0.73125

Alpha virt. eigenvalues -- 0.73242 0.73484 0.74077 0.74472 0.74663

Alpha virt. eigenvalues -- 0.75573 0.75651 0.75767 0.75821 0.76211

Alpha virt. eigenvalues -- 0.76432 0.76727 0.77083 0.77785 0.77986

Alpha virt. eigenvalues -- 0.78017 0.78212 0.78803 0.79415 0.79571

Alpha virt. eigenvalues -- 0.79672 0.79679 0.80291 0.80409 0.80832

Alpha virt. eigenvalues -- 0.81393 0.82042 0.82127 0.82549 0.83492

Alpha virt. eigenvalues -- 0.83817 0.84467 0.85208 0.86209 0.86374

Alpha virt. eigenvalues -- 0.86601 0.87228 0.87453 0.87929 0.87987

Alpha virt. eigenvalues -- 0.88176 0.88338 0.89955 0.90336 0.91001

Alpha virt. eigenvalues -- 0.91365 0.91641 0.91971 0.92584 0.92795

Alpha virt. eigenvalues -- 0.93197 0.94343 0.94677 0.94687 0.95028

Alpha virt. eigenvalues -- 0.95643 0.95800 0.96566 0.97903 0.98347

Alpha virt. eigenvalues -- 0.99270 0.99936 1.00513 1.00671 1.00709

Alpha virt. eigenvalues -- 1.00793 1.01577 1.02004 1.02312 1.02861

Alpha virt. eigenvalues -- 1.03079 1.03977 1.05040 1.05912 1.06778

Alpha virt. eigenvalues -- 1.07669 1.07897 1.08008 1.08411 1.09093

Alpha virt. eigenvalues -- 1.09556 1.11218 1.12069 1.12115 1.12242

Alpha virt. eigenvalues -- 1.12534 1.13448 1.13691 1.14113 1.14339

Alpha virt. eigenvalues -- 1.14880 1.14947 1.15161 1.15253 1.15950

Alpha virt. eigenvalues -- 1.17494 1.17709 1.17811 1.18560 1.18624

Alpha virt. eigenvalues -- 1.19417 1.19519 1.19586 1.19885 1.19968

Alpha virt. eigenvalues -- 1.20260 1.21074 1.22189 1.22395 1.22503

Alpha virt. eigenvalues -- 1.23689 1.24053 1.24075 1.24248 1.24422

Alpha virt. eigenvalues -- 1.24765 1.25016 1.25223 1.26516 1.27124

Alpha virt. eigenvalues -- 1.27461 1.27510 1.28428 1.28537 1.29884

Alpha virt. eigenvalues -- 1.31021 1.31289 1.31309 1.32167 1.33202

Alpha virt. eigenvalues -- 1.34576 1.35783 1.36775 1.38224 1.38226

Alpha virt. eigenvalues -- 1.38715 1.40016 1.40956 1.41379 1.41432

Alpha virt. eigenvalues -- 1.41974 1.43596 1.43822 1.44375 1.44689

Alpha virt. eigenvalues -- 1.45483 1.46030 1.46341 1.46434 1.46833

Alpha virt. eigenvalues -- 1.46858 1.46880 1.47472 1.48219 1.48405

Alpha virt. eigenvalues -- 1.48590 1.50710 1.51908 1.52080 1.52321

Alpha virt. eigenvalues -- 1.52350 1.52522 1.52885 1.52911 1.54302

Alpha virt. eigenvalues -- 1.55677 1.56309 1.57197 1.60138 1.60347

Alpha virt. eigenvalues -- 1.60709 1.60934 1.61139 1.61928 1.63566

Alpha virt. eigenvalues -- 1.63729 1.65554 1.66056 1.66406 1.66590

Alpha virt. eigenvalues -- 1.67153 1.67783 1.68313 1.68656 1.69201

Alpha virt. eigenvalues -- 1.69873 1.70099 1.72071 1.72341 1.73168

Alpha virt. eigenvalues -- 1.73278 1.73637 1.73765 1.74128 1.74731

Alpha virt. eigenvalues -- 1.74960 1.75694 1.76360 1.76997 1.77812

Alpha virt. eigenvalues -- 1.78017 1.78926 1.79222 1.79251 1.79604

Alpha virt. eigenvalues -- 1.80174 1.80211 1.80345 1.80763 1.81444

Alpha virt. eigenvalues -- 1.81694 1.82480 1.83131 1.83143 1.83888

Alpha virt. eigenvalues -- 1.84091 1.84339 1.86011 1.86335 1.86699

Alpha virt. eigenvalues -- 1.87074 1.87464 1.87674 1.88353 1.89110

Alpha virt. eigenvalues -- 1.89419 1.90656 1.90888 1.91157 1.91192

Alpha virt. eigenvalues -- 1.91395 1.91773 1.91778 1.91894 1.92269

Alpha virt. eigenvalues -- 1.92511 1.92588 1.92755 1.93007 1.93380

Alpha virt. eigenvalues -- 1.93463 1.93539 1.94779 1.94865 1.94921

Alpha virt. eigenvalues -- 1.95028 1.95274 1.96044 1.96118 1.96332

Alpha virt. eigenvalues -- 1.98010 1.98450 1.99481 1.99694 2.00566

Alpha virt. eigenvalues -- 2.00763 2.04039 2.05101 2.05231 2.06825

Alpha virt. eigenvalues -- 2.07223 2.07647 2.08831 2.09462 2.12179

Alpha virt. eigenvalues -- 2.12405 2.12492 2.15382 2.16974 2.20663

Alpha virt. eigenvalues -- 2.22503 2.22531 2.23082 2.23522 2.23679

Alpha virt. eigenvalues -- 2.24127 2.24495 2.24555 2.25068 2.25188

Alpha virt. eigenvalues -- 2.26273 2.26279 2.26742 2.26762 2.26956

Alpha virt. eigenvalues -- 2.27049 2.27077 2.27213 2.27805 2.28818

Alpha virt. eigenvalues -- 2.28900 2.28944 2.29665 2.30089 2.30454

Alpha virt. eigenvalues -- 2.31081 2.31650 2.31929 2.32065 2.33608

Alpha virt. eigenvalues -- 2.33772 2.33968 2.34751 2.34958 2.35521

Alpha virt. eigenvalues -- 2.35583 2.36307 2.37018 2.37215 2.37596

Alpha virt. eigenvalues -- 2.38536 2.38569 2.39810 2.41870 2.41976

Alpha virt. eigenvalues -- 2.43162 2.43440 2.45793 2.46752 2.46945

Alpha virt. eigenvalues -- 2.49313 2.50044 2.50489 2.51209 2.51266

Alpha virt. eigenvalues -- 2.52885 2.54266 2.55833 2.56072 2.56635

Alpha virt. eigenvalues -- 2.57003 2.57728 2.58281 2.58423 2.58453

Alpha virt. eigenvalues -- 2.59516 2.60279 2.60323 2.61181 2.62643

Alpha virt. eigenvalues -- 2.63947 2.64814 2.65179 2.65520 2.66245

Alpha virt. eigenvalues -- 2.66298 2.69180 2.69554 2.69594 2.69903

Alpha virt. eigenvalues -- 2.69964 2.71180 2.71266 2.71470 2.72526

Alpha virt. eigenvalues -- 2.72968 2.73995 2.74171 2.75329 2.75586

Alpha virt. eigenvalues -- 2.76034 2.77098 2.77480 2.77626 2.77773

Alpha virt. eigenvalues -- 2.78398 2.81597 2.81940 2.82232 2.82264

Alpha virt. eigenvalues -- 2.82390 2.84151 2.84627 2.85270 2.86285

Alpha virt. eigenvalues -- 2.87408 2.88311 2.89013 2.89293 2.91261

Alpha virt. eigenvalues -- 2.93223 2.94311 2.94620 2.96378 2.96469

Alpha virt. eigenvalues -- 2.97259 2.97544 2.98046 3.00286 3.01236

Alpha virt. eigenvalues -- 3.01656 3.01667 3.02834 3.04027 3.04454

Alpha virt. eigenvalues -- 3.06040 3.06258 3.06383 3.06706 3.06932

Alpha virt. eigenvalues -- 3.08883 3.08906 3.11102 3.11443 3.13274

Alpha virt. eigenvalues -- 3.14187 3.14256 3.14812 3.15485 3.17496

Alpha virt. eigenvalues -- 3.17938 3.18265 3.20447 3.20902 3.21615

Alpha virt. eigenvalues -- 3.23724 3.25266 3.25562 3.25719 3.25858

Alpha virt. eigenvalues -- 3.26529 3.28490 3.28543 3.28664 3.29233

Alpha virt. eigenvalues -- 3.29547 3.29885 3.30220 3.30229 3.30274

Alpha virt. eigenvalues -- 3.30579 3.30898 3.31031 3.31140 3.32007

Alpha virt. eigenvalues -- 3.32358 3.32601 3.33411 3.33618 3.34634

Alpha virt. eigenvalues -- 3.35153 3.36515 3.36576 3.38363 3.39210

Alpha virt. eigenvalues -- 3.40835 3.42400 3.42793 3.43123 3.44666

Alpha virt. eigenvalues -- 3.47932 3.49806 3.50064 3.50609 3.56115

Alpha virt. eigenvalues -- 3.56525 3.57334 3.57722 3.57772 3.59377

Alpha virt. eigenvalues -- 3.59671 3.59722 3.60570 3.63392 3.63842

Alpha virt. eigenvalues -- 3.65623 3.70531 3.70546 3.71126 3.73359

Alpha virt. eigenvalues -- 3.75012 3.77041 3.78826 3.79642 3.82082

Alpha virt. eigenvalues -- 3.83146 3.85321 3.88259 3.89747 3.91871

Alpha virt. eigenvalues -- 3.92262 3.93060 3.94421 3.94886 3.95747

Alpha virt. eigenvalues -- 3.95972 3.97453 3.98070 4.01153 4.09145

Alpha virt. eigenvalues -- 4.27408 4.28612 4.34905 4.38353 4.46221

Alpha virt. eigenvalues -- 4.50145 4.53054 4.53445 4.61545 4.61685

Alpha virt. eigenvalues -- 4.64706 4.65878 4.77784 4.77799 4.77805

Alpha virt. eigenvalues -- 4.77823 5.07421 5.13733 5.15501 5.25839

Alpha virt. eigenvalues -- 23.23913 23.27560 23.27732 23.29482 23.44543

Alpha virt. eigenvalues -- 23.51004 23.51646 23.56900 23.72380 23.73407

Alpha virt. eigenvalues -- 23.76021 23.77202 23.79665 23.79851 23.79864

Alpha virt. eigenvalues -- 23.80146 23.84727 23.85468 23.85519 23.86156

Alpha virt. eigenvalues -- 23.90315 23.90617 23.93952 23.95641 23.96054

Alpha virt. eigenvalues -- 23.97081 23.97635 23.97886 24.04350 24.04467

Alpha virt. eigenvalues -- 24.04549 24.04649 24.05501 24.05768 24.06321

Alpha virt. eigenvalues -- 24.06545 24.10287 24.10384 24.14430 24.14458

Alpha virt. eigenvalues -- 24.14461 24.14474 24.15050 24.15206 35.54124

Alpha virt. eigenvalues -- 35.55004 35.61098 35.61647

Beta occ. eigenvalues -- -14.37940 -14.37940 -14.31511 -14.31511 -10.24473

Beta occ. eigenvalues -- -10.24473 -10.24473 -10.24472 -10.23153 -10.23153

Beta occ. eigenvalues -- -10.23153 -10.23153 -10.22489 -10.22489 -10.22489

Beta occ. eigenvalues -- -10.22489 -10.20062 -10.20062 -10.20062 -10.20062

Beta occ. eigenvalues -- -10.19311 -10.19310 -10.19249 -10.19249 -10.18471

Beta occ. eigenvalues -- -10.18471 -10.18470 -10.18470 -10.18437 -10.18437

Beta occ. eigenvalues -- -10.18437 -10.18437 -10.18189 -10.18189 -10.18189

Beta occ. eigenvalues -- -10.18189 -10.18007 -10.18007 -10.18007 -10.18007

Beta occ. eigenvalues -- -10.17997 -10.17997 -10.17997 -10.17997 -10.17911

Beta occ. eigenvalues -- -10.17911 -10.17841 -10.17841 -1.01658 -1.01514

Beta occ. eigenvalues -- -0.96901 -0.96623 -0.88509 -0.87916 -0.87862

Beta occ. eigenvalues -- -0.87604 -0.84342 -0.83022 -0.82594 -0.81740

Beta occ. eigenvalues -- -0.81226 -0.80017 -0.78027 -0.77623 -0.76168

Beta occ. eigenvalues -- -0.75854 -0.75823 -0.75786 -0.75630 -0.75233

Beta occ. eigenvalues -- -0.74728 -0.74237 -0.72439 -0.68746 -0.68154

Beta occ. eigenvalues -- -0.63910 -0.62748 -0.62404 -0.62103 -0.62014

Beta occ. eigenvalues -- -0.61638 -0.61600 -0.61582 -0.61264 -0.60939

Beta occ. eigenvalues -- -0.60689 -0.59436 -0.58802 -0.57687 -0.56972

Beta occ. eigenvalues -- -0.56272 -0.54396 -0.53614 -0.53281 -0.52461

Beta occ. eigenvalues -- -0.52397 -0.51389 -0.51244 -0.50315 -0.48067

Beta occ. eigenvalues -- -0.47871 -0.47148 -0.46966 -0.46908 -0.46806

Beta occ. eigenvalues -- -0.46449 -0.46341 -0.46181 -0.45595 -0.45577

Beta occ. eigenvalues -- -0.44892 -0.44491 -0.44170 -0.43812 -0.43782

Beta occ. eigenvalues -- -0.43464 -0.43223 -0.43102 -0.43016 -0.42992

Beta occ. eigenvalues -- -0.42979 -0.42251 -0.41748 -0.41129 -0.41093

Beta occ. eigenvalues -- -0.40979 -0.40003 -0.39742 -0.39613 -0.39037

Beta occ. eigenvalues -- -0.37844 -0.37825 -0.37599 -0.37338 -0.36234

Beta occ. eigenvalues -- -0.35941 -0.35793 -0.35568 -0.35478 -0.35469

Beta occ. eigenvalues -- -0.35449 -0.35427 -0.33460 -0.30598 -0.30060

Beta occ. eigenvalues -- -0.29928 -0.29779 -0.28392 -0.28365 -0.27609

Beta occ. eigenvalues -- -0.26754 -0.26735 -0.26678 -0.26579 -0.26165

Beta occ. eigenvalues -- -0.26088 -0.25747 -0.25652 -0.25507 -0.22670

Beta virt. eigenvalues -- -0.17078 -0.10482 -0.10451 -0.05257 -0.02348

Beta virt. eigenvalues -- -0.02323 -0.02169 -0.01880 -0.01766 -0.01703

Beta virt. eigenvalues -- -0.01663 -0.01616 0.01218 0.03644 0.04095

Beta virt. eigenvalues -- 0.04928 0.05338 0.05356 0.05470 0.05824

Beta virt. eigenvalues -- 0.06723 0.07812 0.07881 0.08056 0.08950

Beta virt. eigenvalues -- 0.09086 0.09157 0.09205 0.09384 0.09550

Beta virt. eigenvalues -- 0.09784 0.09883 0.10084 0.10161 0.10343

Beta virt. eigenvalues -- 0.10518 0.11128 0.12226 0.12228 0.12379

Beta virt. eigenvalues -- 0.12402 0.12730 0.12844 0.12854 0.13415

Beta virt. eigenvalues -- 0.13943 0.13964 0.14014 0.14182 0.14426

Beta virt. eigenvalues -- 0.14986 0.15264 0.15330 0.15974 0.16502

Beta virt. eigenvalues -- 0.17381 0.19940 0.20187 0.20909 0.21004

Beta virt. eigenvalues -- 0.22491 0.22498 0.22703 0.23303 0.23980

Beta virt. eigenvalues -- 0.24406 0.24659 0.24891 0.25107 0.25139

Beta virt. eigenvalues -- 0.25857 0.26792 0.26929 0.27295 0.27393

Beta virt. eigenvalues -- 0.27418 0.27555 0.28045 0.28165 0.28688

Beta virt. eigenvalues -- 0.28796 0.29025 0.29046 0.29201 0.29764

Beta virt. eigenvalues -- 0.30031 0.30175 0.30264 0.30518 0.30889

Beta virt. eigenvalues -- 0.32152 0.32902 0.33388 0.33974 0.34096

Beta virt. eigenvalues -- 0.34446 0.34630 0.35078 0.35293 0.35374

Beta virt. eigenvalues -- 0.35880 0.36141 0.36212 0.36224 0.36595

Beta virt. eigenvalues -- 0.36679 0.37020 0.37435 0.37486 0.37586

Beta virt. eigenvalues -- 0.38207 0.38400 0.38668 0.39185 0.39316

Beta virt. eigenvalues -- 0.39664 0.39713 0.40063 0.40138 0.40330

Beta virt. eigenvalues -- 0.40418 0.40595 0.40964 0.41073 0.41129

Beta virt. eigenvalues -- 0.41146 0.41251 0.42034 0.42046 0.42137

Beta virt. eigenvalues -- 0.42236 0.42569 0.42896 0.42915 0.42922

Beta virt. eigenvalues -- 0.43769 0.43891 0.44072 0.44209 0.44271

Beta virt. eigenvalues -- 0.44443 0.44601 0.44660 0.44761 0.44835

Beta virt. eigenvalues -- 0.44849 0.45003 0.45812 0.46065 0.46304

Beta virt. eigenvalues -- 0.46523 0.46631 0.46657 0.47274 0.47818

Beta virt. eigenvalues -- 0.48024 0.48394 0.48703 0.49371 0.49558

Beta virt. eigenvalues -- 0.49736 0.50109 0.50293 0.50818 0.51762

Beta virt. eigenvalues -- 0.51909 0.52160 0.52342 0.52999 0.53151

Beta virt. eigenvalues -- 0.53303 0.53609 0.53847 0.54736 0.54811

Beta virt. eigenvalues -- 0.56526 0.56685 0.56863 0.56873 0.57194

Beta virt. eigenvalues -- 0.57378 0.57645 0.58426 0.58678 0.58775

Beta virt. eigenvalues -- 0.59151 0.59364 0.59380 0.59385 0.59511

Beta virt. eigenvalues -- 0.60192 0.60246 0.60262 0.60358 0.60592

Beta virt. eigenvalues -- 0.60897 0.60915 0.61066 0.61082 0.61424

Beta virt. eigenvalues -- 0.61491 0.62018 0.62152 0.62300 0.62822

Beta virt. eigenvalues -- 0.63005 0.63692 0.63843 0.63987 0.64399

Beta virt. eigenvalues -- 0.64413 0.64596 0.64730 0.64947 0.65410

Beta virt. eigenvalues -- 0.65458 0.65566 0.66451 0.66958 0.67199

Beta virt. eigenvalues -- 0.67819 0.67985 0.68186 0.68930 0.68973

Beta virt. eigenvalues -- 0.69051 0.70250 0.70847 0.71155 0.71424

Beta virt. eigenvalues -- 0.71806 0.71852 0.72434 0.72845 0.72866

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Beta virt. eigenvalues -- 0.74678 0.75648 0.75681 0.75809 0.75825

Beta virt. eigenvalues -- 0.76380 0.76467 0.77046 0.77280 0.77879

Beta virt. eigenvalues -- 0.78014 0.78071 0.78274 0.78844 0.79470

Beta virt. eigenvalues -- 0.79647 0.79709 0.79804 0.80431 0.80484

Beta virt. eigenvalues -- 0.80903 0.81407 0.82238 0.82254 0.82585

Beta virt. eigenvalues -- 0.83732 0.83859 0.84491 0.85238 0.86287

Beta virt. eigenvalues -- 0.86434 0.86670 0.87365 0.87529 0.88009

Beta virt. eigenvalues -- 0.88019 0.88265 0.88363 0.90033 0.90453

Beta virt. eigenvalues -- 0.91063 0.91438 0.91686 0.92113 0.92688

Beta virt. eigenvalues -- 0.92933 0.93288 0.94456 0.94721 0.94774

Beta virt. eigenvalues -- 0.95094 0.95702 0.95918 0.96595 0.97941

Beta virt. eigenvalues -- 0.98445 0.99336 0.99996 1.00575 1.00750

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Beta virt. eigenvalues -- 1.06942 1.07859 1.07995 1.08130 1.08471

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Beta virt. eigenvalues -- 1.12290 1.12624 1.13518 1.13737 1.14155

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Beta virt. eigenvalues -- 1.27214 1.27557 1.27595 1.28589 1.28635

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Beta virt. eigenvalues -- 1.33246 1.34597 1.35891 1.36909 1.38420

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Beta virt. eigenvalues -- 1.41455 1.42140 1.43753 1.43906 1.44506

Beta virt. eigenvalues -- 1.44920 1.45587 1.46122 1.46426 1.46534

Beta virt. eigenvalues -- 1.46902 1.46911 1.46993 1.47540 1.48286

Beta virt. eigenvalues -- 1.48485 1.48693 1.50780 1.52015 1.52167

Beta virt. eigenvalues -- 1.52384 1.52445 1.52807 1.52963 1.53011

Beta virt. eigenvalues -- 1.54402 1.55918 1.56574 1.57238 1.60322

Beta virt. eigenvalues -- 1.60397 1.60780 1.61015 1.61203 1.61995

Beta virt. eigenvalues -- 1.63631 1.63798 1.65790 1.66202 1.66502

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Beta virt. eigenvalues -- 1.73209 1.73492 1.73775 1.73830 1.74232

Beta virt. eigenvalues -- 1.74822 1.75007 1.75868 1.76538 1.76970

Beta virt. eigenvalues -- 1.77846 1.78249 1.78982 1.79110 1.79277

Beta virt. eigenvalues -- 1.79642 1.80140 1.80302 1.80362 1.80826

Beta virt. eigenvalues -- 1.81479 1.81736 1.82578 1.83139 1.83202

Beta virt. eigenvalues -- 1.83965 1.84178 1.84376 1.86091 1.86425

Beta virt. eigenvalues -- 1.87023 1.87177 1.87530 1.87841 1.88414

Beta virt. eigenvalues -- 1.89174 1.89758 1.90678 1.90951 1.91214

Beta virt. eigenvalues -- 1.91270 1.91465 1.91808 1.91827 1.91944

Beta virt. eigenvalues -- 1.92325 1.92556 1.92628 1.92809 1.93057

Beta virt. eigenvalues -- 1.93406 1.93528 1.93583 1.94869 1.95002

Beta virt. eigenvalues -- 1.95035 1.95049 1.95332 1.96178 1.96197

Beta virt. eigenvalues -- 1.96453 1.98077 1.98537 1.99589 1.99773

Beta virt. eigenvalues -- 2.00666 2.00816 2.04252 2.05259 2.05398

Beta virt. eigenvalues -- 2.06910 2.07417 2.07929 2.08942 2.09569

Beta virt. eigenvalues -- 2.12280 2.12502 2.12542 2.15838 2.16924

Beta virt. eigenvalues -- 2.20706 2.22592 2.22651 2.23182 2.23587

Beta virt. eigenvalues -- 2.23756 2.24312 2.24599 2.24622 2.25190

Beta virt. eigenvalues -- 2.25284 2.26327 2.26406 2.26787 2.26809

Beta virt. eigenvalues -- 2.26993 2.27079 2.27106 2.27247 2.27895

Beta virt. eigenvalues -- 2.28853 2.28947 2.29021 2.29677 2.30190

Beta virt. eigenvalues -- 2.30564 2.31111 2.31687 2.31953 2.32140

Beta virt. eigenvalues -- 2.33782 2.33810 2.34083 2.34962 2.35001

Beta virt. eigenvalues -- 2.35649 2.35702 2.36359 2.37076 2.37364

Beta virt. eigenvalues -- 2.37893 2.38634 2.38683 2.39868 2.42015

Beta virt. eigenvalues -- 2.42159 2.43362 2.43547 2.45954 2.46852

Beta virt. eigenvalues -- 2.47087 2.49537 2.50191 2.50998 2.51544

Beta virt. eigenvalues -- 2.51549 2.52946 2.54561 2.56086 2.56279

Beta virt. eigenvalues -- 2.56762 2.57252 2.57779 2.58413 2.58510

Beta virt. eigenvalues -- 2.58768 2.60016 2.60272 2.60421 2.61179

Beta virt. eigenvalues -- 2.62866 2.64074 2.64933 2.65215 2.65547

Beta virt. eigenvalues -- 2.66482 2.66514 2.69250 2.69626 2.69629

Beta virt. eigenvalues -- 2.70009 2.70038 2.71341 2.71371 2.71653

Beta virt. eigenvalues -- 2.72801 2.73072 2.74027 2.74291 2.75552

Beta virt. eigenvalues -- 2.75723 2.76155 2.77265 2.77548 2.77750

Beta virt. eigenvalues -- 2.77889 2.78495 2.81587 2.81933 2.82285

Beta virt. eigenvalues -- 2.82292 2.82422 2.84022 2.84741 2.85357

Beta virt. eigenvalues -- 2.86363 2.87461 2.88334 2.89030 2.89311

Beta virt. eigenvalues -- 2.91289 2.93262 2.94358 2.94660 2.96554

Beta virt. eigenvalues -- 2.97299 2.97513 2.97565 2.98235 3.00375

Beta virt. eigenvalues -- 3.01283 3.01563 3.02252 3.03325 3.04109

Beta virt. eigenvalues -- 3.04500 3.06280 3.06416 3.06498 3.06818

Beta virt. eigenvalues -- 3.07020 3.08932 3.09258 3.11151 3.11480

Beta virt. eigenvalues -- 3.13310 3.14194 3.14306 3.14924 3.15531

Beta virt. eigenvalues -- 3.17524 3.17957 3.18327 3.20497 3.20909

Beta virt. eigenvalues -- 3.21620 3.23789 3.25281 3.25576 3.25733

Beta virt. eigenvalues -- 3.25898 3.26563 3.28529 3.28575 3.28691

Beta virt. eigenvalues -- 3.29378 3.29564 3.29910 3.30229 3.30238

Beta virt. eigenvalues -- 3.30317 3.30642 3.30909 3.31062 3.31169

Beta virt. eigenvalues -- 3.32047 3.32374 3.32709 3.33574 3.33693

Beta virt. eigenvalues -- 3.34657 3.35282 3.36548 3.36590 3.38387

Beta virt. eigenvalues -- 3.39248 3.40906 3.42432 3.42823 3.43162

Beta virt. eigenvalues -- 3.44684 3.47990 3.49841 3.50114 3.50652

Beta virt. eigenvalues -- 3.56134 3.56554 3.57341 3.57749 3.57795

Beta virt. eigenvalues -- 3.59364 3.59742 3.59752 3.60563 3.63451

Beta virt. eigenvalues -- 3.63870 3.65666 3.70568 3.70619 3.71155

Beta virt. eigenvalues -- 3.73398 3.75247 3.77078 3.78988 3.79705

Beta virt. eigenvalues -- 3.82435 3.83350 3.86555 3.89433 3.89876

Beta virt. eigenvalues -- 3.91981 3.92363 3.93125 3.94541 3.94935

Beta virt. eigenvalues -- 3.95779 3.96008 3.97523 3.98120 4.01264

Beta virt. eigenvalues -- 4.09226 4.27622 4.28853 4.35145 4.38609

Beta virt. eigenvalues -- 4.46423 4.50359 4.53152 4.53648 4.61785

Beta virt. eigenvalues -- 4.61902 4.64790 4.66014 4.77828 4.77843

Beta virt. eigenvalues -- 4.77849 4.77867 5.07514 5.13813 5.15680

Beta virt. eigenvalues -- 5.26008 23.23935 23.27579 23.27751 23.29500

Beta virt. eigenvalues -- 23.44567 23.51004 23.51674 23.56893 23.72454

Beta virt. eigenvalues -- 23.73479 23.76089 23.77282 23.79684 23.79869

Beta virt. eigenvalues -- 23.79882 23.80164 23.84751 23.85491 23.85544

Beta virt. eigenvalues -- 23.86180 23.90243 23.90569 23.93932 23.95576

Beta virt. eigenvalues -- 23.96181 23.97165 23.97707 23.97934 24.04366

Beta virt. eigenvalues -- 24.04484 24.04565 24.04667 24.05564 24.05835

Beta virt. eigenvalues -- 24.06396 24.06622 24.10300 24.10396 24.14448

Beta virt. eigenvalues -- 24.14480 24.14481 24.14496 24.15037 24.15191

Beta virt. eigenvalues -- 35.54269 35.55148 35.61416 35.61966

Condensed to atoms (all electrons):

Atomic-Atomic Spin Densities.

Mulliken charges and spin densities:

1 2

1 C -0.242005 0.009954

2 C 0.346989 -0.043421

3 N -0.675222 0.064634

4 C 0.346989 -0.043421

5 C -0.242005 0.009954

6 C -0.028084 0.233953

7 C 0.209617 -0.075058

8 N -0.470651 0.147349

9 C 0.209617 -0.075058

10 C -0.236759 -0.009191

11 C -0.236759 -0.009191

12 C -0.028084 0.233953

13 C 0.209617 -0.075058

14 C -0.236759 -0.009191

15 C -0.236759 -0.009191

16 C 0.209617 -0.075058

17 N -0.470651 0.147349

18 C -0.028084 0.233953

19 C 0.346989 -0.043421

20 C -0.242005 0.009954

21 C -0.242005 0.009954

22 C 0.346989 -0.043421

23 N -0.675222 0.064634

24 C -0.028084 0.233953

25 C -0.108977 -0.023192

26 C -0.204205 0.025000

27 C -0.212190 -0.011487

28 C -0.206170 0.026784

29 C -0.212191 -0.011060

30 C -0.201857 0.024897

31 C -0.206170 0.026784

32 C -0.212190 -0.011487

33 C -0.204205 0.025000

34 C -0.108977 -0.023192

35 C -0.201857 0.024897

36 C -0.212191 -0.011060

37 C -0.108977 -0.023192

38 C -0.201857 0.024897

39 C -0.212191 -0.011060

40 C -0.206170 0.026784

41 C -0.212190 -0.011487

42 C -0.204205 0.025000

43 C -0.108977 -0.023192

44 C -0.201857 0.024897

45 C -0.212191 -0.011060

46 C -0.206170 0.026784

47 C -0.212190 -0.011487

48 C -0.204205 0.025000

49 H 0.268086 -0.000208

50 H 0.268086 -0.000208

51 H 0.252782 0.000631

52 H 0.252782 0.000631

53 H 0.252782 0.000631

54 H 0.252782 0.000631

55 H 0.268086 -0.000208

56 H 0.268086 -0.000208

57 H 0.241619 -0.001247

58 H 0.233279 0.000793

59 H 0.233725 -0.001388

60 H 0.233326 0.000793

61 H 0.241114 -0.001139

62 H 0.233725 -0.001388

63 H 0.233279 0.000793

64 H 0.241619 -0.001247

65 H 0.241114 -0.001139

66 H 0.233326 0.000793

67 H 0.241114 -0.001139

68 H 0.233326 0.000793

69 H 0.233725 -0.001388

70 H 0.233279 0.000793

71 H 0.241619 -0.001247

72 H 0.241114 -0.001139

73 H 0.233326 0.000793

74 H 0.233725 -0.001388

75 H 0.233279 0.000793

76 H 0.241619 -0.001247

77 H 0.429671 -0.002805

78 H 0.429671 -0.002805

Sum of Mulliken charges = 1.00000 1.00000

Mulliken charges and spin densities with hydrogens summed into heavy atoms:

1 2

1 C 0.026081 0.009746

2 C 0.346989 -0.043421

3 N -0.245550 0.061829

4 C 0.346989 -0.043421

5 C 0.026081 0.009746

6 C -0.028084 0.233953

7 C 0.209617 -0.075058

8 N -0.470651 0.147349

9 C 0.209617 -0.075058

10 C 0.016024 -0.008560

11 C 0.016024 -0.008560

12 C -0.028084 0.233953

13 C 0.209617 -0.075058

14 C 0.016024 -0.008560

15 C 0.016024 -0.008560

16 C 0.209617 -0.075058

17 N -0.470651 0.147349

18 C -0.028084 0.233953

19 C 0.346989 -0.043421

20 C 0.026081 0.009746

21 C 0.026081 0.009746

22 C 0.346989 -0.043421

23 N -0.245550 0.061829

24 C -0.028084 0.233953

25 C -0.108977 -0.023192

26 C 0.037414 0.023752

27 C 0.021088 -0.010693

28 C 0.027556 0.025395

29 C 0.021135 -0.010267

30 C 0.039256 0.023757

31 C 0.027556 0.025395

32 C 0.021088 -0.010693

33 C 0.037414 0.023752

34 C -0.108977 -0.023192

35 C 0.039256 0.023757

36 C 0.021135 -0.010267

37 C -0.108977 -0.023192

38 C 0.039256 0.023757

39 C 0.021135 -0.010267

40 C 0.027556 0.025395

41 C 0.021088 -0.010693

42 C 0.037414 0.023752

43 C -0.108977 -0.023192

44 C 0.039256 0.023757

45 C 0.021135 -0.010267

46 C 0.027556 0.025395

47 C 0.021088 -0.010693

48 C 0.037414 0.023752

Electronic spatial extent (au): <R\*\*2>= 32902.8541

Charge= 1.0000 electrons

Dipole moment (field-independent basis, Debye):

X= -0.0000 Y= 0.0000 Z= -0.5402 Tot= 0.5402

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -170.3276 YY= -152.7827 ZZ= -268.6373

XY= -0.0000 XZ= 0.0000 YZ= 0.0000

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= 26.9216 YY= 44.4665 ZZ= -71.3881

XY= -0.0000 XZ= 0.0000 YZ= 0.0000

Octapole moment (field-independent basis, Debye-Ang\*\*2):

XXX= 0.0000 YYY= -0.0000 ZZZ= 0.9586 XYY= 0.0000

XXY= -0.0000 XXZ= 104.1557 XZZ= 0.0000 YZZ= -0.0000

YYZ= -90.1742 XYZ= -0.0000

Hexadecapole moment (field-independent basis, Debye-Ang\*\*3):

XXXX= -19343.5359 YYYY= -18728.0212 ZZZZ= -965.4891 XXXY= 0.0000

XXXZ= -0.0000 YYYX= 0.0000 YYYZ= 0.0000 ZZZX= -0.0000

ZZZY= -0.0000 XXYY= -4735.2090 XXZZ= -3837.9227 YYZZ= -3782.5539

XXYZ= -0.0000 YYXZ= -0.0000 ZZXY= -0.0000

N-N= 5.372013261903D+03 E-N=-1.515861334761D+04 KE= 1.906181753880D+03

Symmetry A1 KE= 5.306577379624D+02

Symmetry A2 KE= 4.230403942546D+02

Symmetry B1 KE= 4.763394355580D+02

Symmetry B2 KE= 4.761441861046D+02

Isotropic Fermi Contact Couplings

Atom a.u. MegaHertz Gauss 10(-4) cm-1

1 C(13) 0.00051 0.57020 0.20346 0.19020

2 C(13) -0.01014 -11.40423 -4.06931 -3.80404

3 N(14) 0.00802 2.59101 0.92454 0.86427

4 C(13) -0.01014 -11.40423 -4.06931 -3.80404

5 C(13) 0.00051 0.57020 0.20346 0.19020

6 C(13) 0.01430 16.07825 5.73712 5.36313

7 C(13) -0.01297 -14.58494 -5.20427 -4.86501

8 N(14) 0.01431 4.62208 1.64927 1.54176

9 C(13) -0.01297 -14.58494 -5.20427 -4.86501

10 C(13) 0.00036 0.40371 0.14405 0.13466

11 C(13) 0.00036 0.40371 0.14405 0.13466

12 C(13) 0.01430 16.07825 5.73712 5.36313

13 C(13) -0.01297 -14.58494 -5.20427 -4.86501

14 C(13) 0.00036 0.40371 0.14405 0.13466

15 C(13) 0.00036 0.40371 0.14405 0.13466

16 C(13) -0.01297 -14.58494 -5.20427 -4.86501

17 N(14) 0.01431 4.62208 1.64927 1.54176

18 C(13) 0.01430 16.07825 5.73712 5.36313

19 C(13) -0.01014 -11.40423 -4.06931 -3.80404

20 C(13) 0.00051 0.57020 0.20346 0.19020

21 C(13) 0.00051 0.57020 0.20346 0.19020

22 C(13) -0.01014 -11.40423 -4.06931 -3.80404

23 N(14) 0.00802 2.59101 0.92454 0.86427

24 C(13) 0.01430 16.07825 5.73712 5.36313

25 C(13) -0.00784 -8.81106 -3.14401 -2.93905

26 C(13) 0.00708 7.95398 2.83818 2.65316

27 C(13) -0.00084 -0.94788 -0.33823 -0.31618

28 C(13) 0.00161 1.80671 0.64468 0.60265

29 C(13) -0.00075 -0.84510 -0.30155 -0.28189

30 C(13) 0.00756 8.50045 3.03317 2.83545

31 C(13) 0.00161 1.80671 0.64468 0.60265

32 C(13) -0.00084 -0.94788 -0.33823 -0.31618

33 C(13) 0.00708 7.95398 2.83818 2.65316

34 C(13) -0.00784 -8.81106 -3.14401 -2.93905

35 C(13) 0.00756 8.50045 3.03317 2.83545

36 C(13) -0.00075 -0.84510 -0.30155 -0.28189

37 C(13) -0.00784 -8.81106 -3.14401 -2.93905

38 C(13) 0.00756 8.50045 3.03317 2.83545

39 C(13) -0.00075 -0.84510 -0.30155 -0.28189

40 C(13) 0.00161 1.80671 0.64468 0.60265

41 C(13) -0.00084 -0.94788 -0.33823 -0.31618

42 C(13) 0.00708 7.95398 2.83818 2.65316

43 C(13) -0.00784 -8.81106 -3.14401 -2.93905

44 C(13) 0.00756 8.50045 3.03317 2.83545

45 C(13) -0.00075 -0.84510 -0.30155 -0.28189

46 C(13) 0.00161 1.80671 0.64468 0.60265

47 C(13) -0.00084 -0.94788 -0.33823 -0.31618

48 C(13) 0.00708 7.95398 2.83818 2.65316

49 H(1) -0.00011 -0.47733 -0.17032 -0.15922

50 H(1) -0.00011 -0.47733 -0.17032 -0.15922

51 H(1) 0.00018 0.81675 0.29144 0.27244

52 H(1) 0.00018 0.81675 0.29144 0.27244

53 H(1) 0.00018 0.81675 0.29144 0.27244

54 H(1) 0.00018 0.81675 0.29144 0.27244

55 H(1) -0.00011 -0.47733 -0.17032 -0.15922

56 H(1) -0.00011 -0.47733 -0.17032 -0.15922

57 H(1) -0.00040 -1.79468 -0.64039 -0.59864

58 H(1) 0.00026 1.14152 0.40732 0.38077

59 H(1) -0.00038 -1.67836 -0.59888 -0.55984

60 H(1) 0.00026 1.17084 0.41778 0.39055

61 H(1) -0.00040 -1.78203 -0.63587 -0.59442

62 H(1) -0.00038 -1.67836 -0.59888 -0.55984

63 H(1) 0.00026 1.14152 0.40732 0.38077

64 H(1) -0.00040 -1.79468 -0.64039 -0.59864

65 H(1) -0.00040 -1.78203 -0.63587 -0.59442

66 H(1) 0.00026 1.17084 0.41778 0.39055

67 H(1) -0.00040 -1.78203 -0.63587 -0.59442

68 H(1) 0.00026 1.17084 0.41778 0.39055

69 H(1) -0.00038 -1.67836 -0.59888 -0.55984

70 H(1) 0.00026 1.14152 0.40732 0.38077

71 H(1) -0.00040 -1.79468 -0.64039 -0.59864

72 H(1) -0.00040 -1.78203 -0.63587 -0.59442

73 H(1) 0.00026 1.17084 0.41778 0.39055

74 H(1) -0.00038 -1.67836 -0.59888 -0.55984

75 H(1) 0.00026 1.14152 0.40732 0.38077

76 H(1) -0.00040 -1.79468 -0.64039 -0.59864

77 H(1) -0.00100 -4.48377 -1.59992 -1.49562

78 H(1) -0.00100 -4.48377 -1.59992 -1.49562

--------------------------------------------------------

Center ---- Spin Dipole Couplings ----

3XX-RR 3YY-RR 3ZZ-RR

--------------------------------------------------------

1 Atom -0.003046 0.000334 0.002712

2 Atom 0.023882 0.010349 -0.034231

3 Atom -0.072718 -0.054995 0.127712

4 Atom 0.023882 0.010349 -0.034231

5 Atom -0.003046 0.000334 0.002712

6 Atom -0.127541 -0.127452 0.254993

7 Atom 0.023497 0.042356 -0.065852

8 Atom -0.136541 -0.163808 0.300350

9 Atom 0.023497 0.042356 -0.065852

10 Atom 0.008677 0.007451 -0.016128

11 Atom 0.008677 0.007451 -0.016128

12 Atom -0.127541 -0.127452 0.254993

13 Atom 0.023497 0.042356 -0.065852

14 Atom 0.008677 0.007451 -0.016128

15 Atom 0.008677 0.007451 -0.016128

16 Atom 0.023497 0.042356 -0.065852

17 Atom -0.136541 -0.163808 0.300350

18 Atom -0.127541 -0.127452 0.254993

19 Atom 0.023882 0.010349 -0.034231

20 Atom -0.003046 0.000334 0.002712

21 Atom -0.003046 0.000334 0.002712

22 Atom 0.023882 0.010349 -0.034231

23 Atom -0.072718 -0.054995 0.127712

24 Atom -0.127541 -0.127452 0.254993

25 Atom -0.001869 -0.001960 0.003829

26 Atom -0.008434 0.016349 -0.007915

27 Atom 0.000412 0.002807 -0.003218

28 Atom -0.002229 -0.002642 0.004871

29 Atom 0.003135 0.000213 -0.003348

30 Atom 0.017324 -0.009176 -0.008149

31 Atom -0.002229 -0.002642 0.004871

32 Atom 0.000412 0.002807 -0.003218

33 Atom -0.008434 0.016349 -0.007915

34 Atom -0.001869 -0.001960 0.003829

35 Atom 0.017324 -0.009176 -0.008149

36 Atom 0.003135 0.000213 -0.003348

37 Atom -0.001869 -0.001960 0.003829

38 Atom 0.017324 -0.009176 -0.008149

39 Atom 0.003135 0.000213 -0.003348

40 Atom -0.002229 -0.002642 0.004871

41 Atom 0.000412 0.002807 -0.003218

42 Atom -0.008434 0.016349 -0.007915

43 Atom -0.001869 -0.001960 0.003829

44 Atom 0.017324 -0.009176 -0.008149

45 Atom 0.003135 0.000213 -0.003348

46 Atom -0.002229 -0.002642 0.004871

47 Atom 0.000412 0.002807 -0.003218

48 Atom -0.008434 0.016349 -0.007915

49 Atom 0.000439 0.000993 -0.001432

50 Atom 0.000439 0.000993 -0.001432

51 Atom 0.001035 0.000077 -0.001112

52 Atom 0.001035 0.000077 -0.001112

53 Atom 0.001035 0.000077 -0.001112

54 Atom 0.001035 0.000077 -0.001112

55 Atom 0.000439 0.000993 -0.001432

56 Atom 0.000439 0.000993 -0.001432

57 Atom -0.000125 0.000745 -0.000620

58 Atom 0.000132 0.000187 -0.000318

59 Atom 0.000729 0.000670 -0.001399

60 Atom 0.000235 0.000057 -0.000292

61 Atom 0.000883 -0.000132 -0.000751

62 Atom 0.000729 0.000670 -0.001399

63 Atom 0.000132 0.000187 -0.000318

64 Atom -0.000125 0.000745 -0.000620

65 Atom 0.000883 -0.000132 -0.000751

66 Atom 0.000235 0.000057 -0.000292

67 Atom 0.000883 -0.000132 -0.000751

68 Atom 0.000235 0.000057 -0.000292

69 Atom 0.000729 0.000670 -0.001399

70 Atom 0.000132 0.000187 -0.000318

71 Atom -0.000125 0.000745 -0.000620

72 Atom 0.000883 -0.000132 -0.000751

73 Atom 0.000235 0.000057 -0.000292

74 Atom 0.000729 0.000670 -0.001399

75 Atom 0.000132 0.000187 -0.000318

76 Atom -0.000125 0.000745 -0.000620

77 Atom -0.001494 0.006474 -0.004980

78 Atom -0.001494 0.006474 -0.004980

--------------------------------------------------------

XY XZ YZ

--------------------------------------------------------

1 Atom 0.001208 -0.000414 -0.006457

2 Atom 0.001365 -0.000342 0.009832

3 Atom -0.000000 -0.000000 -0.071614

4 Atom -0.001365 0.000342 0.009832

5 Atom -0.001208 0.000414 -0.006457

6 Atom -0.000631 0.034536 -0.036873

7 Atom 0.004119 -0.022972 0.002909

8 Atom 0.000000 0.127777 0.000000

9 Atom -0.004119 -0.022972 -0.002909

10 Atom 0.000532 -0.005868 0.000084

11 Atom -0.000532 -0.005868 -0.000084

12 Atom 0.000631 -0.034536 -0.036873

13 Atom -0.004119 0.022972 0.002909

14 Atom 0.000532 0.005868 -0.000084

15 Atom -0.000532 0.005868 0.000084

16 Atom 0.004119 0.022972 -0.002909

17 Atom 0.000000 -0.127777 -0.000000

18 Atom -0.000631 -0.034536 0.036873

19 Atom -0.001365 -0.000342 -0.009832

20 Atom -0.001208 -0.000414 0.006457

21 Atom 0.001208 0.000414 0.006457

22 Atom 0.001365 0.000342 -0.009832

23 Atom -0.000000 0.000000 0.071614

24 Atom 0.000631 0.034536 0.036873

25 Atom 0.007873 0.006048 -0.005384

26 Atom -0.011964 -0.007479 0.012011

27 Atom 0.005881 0.005906 -0.005072

28 Atom -0.010367 -0.015327 0.015114

29 Atom 0.005738 0.004882 -0.005813

30 Atom -0.011533 -0.011530 0.006744

31 Atom 0.010367 0.015327 0.015114

32 Atom -0.005881 -0.005906 -0.005072

33 Atom 0.011964 0.007479 0.012011

34 Atom -0.007873 -0.006048 -0.005384

35 Atom 0.011533 0.011530 0.006744

36 Atom -0.005738 -0.004882 -0.005813

37 Atom -0.007873 0.006048 0.005384

38 Atom 0.011533 -0.011530 -0.006744

39 Atom -0.005738 0.004882 0.005813

40 Atom 0.010367 -0.015327 -0.015114

41 Atom -0.005881 0.005906 0.005072

42 Atom 0.011964 -0.007479 -0.012011

43 Atom 0.007873 -0.006048 0.005384

44 Atom -0.011533 0.011530 -0.006744

45 Atom 0.005738 -0.004882 0.005813

46 Atom -0.010367 0.015327 -0.015114

47 Atom 0.005881 -0.005906 0.005072

48 Atom -0.011964 0.007479 -0.012011

49 Atom -0.000036 -0.000099 0.000661

50 Atom 0.000036 0.000099 0.000661

51 Atom 0.001428 -0.000538 -0.000532

52 Atom -0.001428 -0.000538 0.000532

53 Atom 0.001428 0.000538 0.000532

54 Atom -0.001428 0.000538 -0.000532

55 Atom 0.000036 -0.000099 -0.000661

56 Atom -0.000036 0.000099 -0.000661

57 Atom -0.000316 0.001187 -0.001968

58 Atom 0.000697 0.000218 -0.000212

59 Atom 0.001807 -0.000540 0.000567

60 Atom 0.000653 0.000229 -0.000253

61 Atom -0.000482 0.001916 -0.001461

62 Atom -0.001807 0.000540 0.000567

63 Atom -0.000697 -0.000218 -0.000212

64 Atom 0.000316 -0.001187 -0.001968

65 Atom 0.000482 -0.001916 -0.001461

66 Atom -0.000653 -0.000229 -0.000253

67 Atom 0.000482 0.001916 0.001461

68 Atom -0.000653 0.000229 0.000253

69 Atom -0.001807 -0.000540 -0.000567

70 Atom -0.000697 0.000218 0.000212

71 Atom 0.000316 0.001187 0.001968

72 Atom -0.000482 -0.001916 0.001461

73 Atom 0.000653 -0.000229 0.000253

74 Atom 0.001807 0.000540 -0.000567

75 Atom 0.000697 -0.000218 0.000212

76 Atom -0.000316 -0.001187 0.001968

77 Atom -0.000000 0.000000 0.003134

78 Atom 0.000000 0.000000 -0.003134

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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 -0.0053 -0.705 -0.251 -0.235 -0.2992 0.7487 0.5916

1 C(13) Bbb -0.0029 -0.395 -0.141 -0.132 0.9493 0.1706 0.2642

Bcc 0.0082 1.100 0.392 0.367 -0.0969 -0.6406 0.7617

Baa -0.0363 -4.872 -1.739 -1.625 0.0102 -0.2065 0.9784

2 C(13) Bbb 0.0123 1.648 0.588 0.550 -0.1084 0.9725 0.2064

Bcc 0.0240 3.224 1.150 1.075 0.9941 0.1081 0.0124

Baa -0.0797 -3.075 -1.097 -1.026 0.0000 0.9453 0.3263

3 N(14) Bbb -0.0727 -2.805 -1.001 -0.935 1.0000 -0.0000 0.0000

Bcc 0.1524 5.879 2.098 1.961 -0.0000 -0.3263 0.9453

Baa -0.0363 -4.872 -1.739 -1.625 -0.0102 -0.2065 0.9784

4 C(13) Bbb 0.0123 1.648 0.588 0.550 0.1084 0.9725 0.2064

Bcc 0.0240 3.224 1.150 1.075 0.9941 -0.1081 -0.0124

Baa -0.0053 -0.705 -0.251 -0.235 0.2992 0.7487 0.5916

5 C(13) Bbb -0.0029 -0.395 -0.141 -0.132 0.9493 -0.1706 -0.2642

Bcc 0.0082 1.100 0.392 0.367 0.0969 -0.6406 0.7617

Baa -0.1334 -17.906 -6.389 -5.973 -0.6783 0.7233 0.1290

6 C(13) Bbb -0.1281 -17.194 -6.135 -5.735 0.7294 0.6840 0.0001

Bcc 0.2616 35.099 12.524 11.708 0.0882 -0.0941 0.9916

Baa -0.0715 -9.600 -3.425 -3.202 0.2362 -0.0333 0.9711

7 C(13) Bbb 0.0283 3.795 1.354 1.266 0.9444 -0.2273 -0.2375

Bcc 0.0433 5.805 2.071 1.936 0.2287 0.9732 -0.0222

Baa -0.1712 -6.602 -2.356 -2.202 0.9652 -0.0000 -0.2616

8 N(14) Bbb -0.1638 -6.318 -2.254 -2.107 0.0000 1.0000 -0.0000

Bcc 0.3350 12.919 4.610 4.309 0.2616 0.0000 0.9652

Baa -0.0715 -9.600 -3.425 -3.202 0.2362 0.0333 0.9711

9 C(13) Bbb 0.0283 3.795 1.354 1.266 0.9444 0.2273 -0.2375

Bcc 0.0433 5.805 2.071 1.936 -0.2287 0.9732 0.0222

Baa -0.0174 -2.341 -0.835 -0.781 0.2193 -0.0080 0.9756

10 C(13) Bbb 0.0074 0.987 0.352 0.329 -0.1803 0.9824 0.0485

Bcc 0.0101 1.354 0.483 0.452 0.9589 0.1865 -0.2140

Baa -0.0174 -2.341 -0.835 -0.781 0.2193 0.0080 0.9756

11 C(13) Bbb 0.0074 0.987 0.352 0.329 0.1803 0.9824 -0.0485

Bcc 0.0101 1.354 0.483 0.452 0.9589 -0.1865 -0.2140

Baa -0.1334 -17.906 -6.389 -5.973 0.6783 0.7233 0.1290

12 C(13) Bbb -0.1281 -17.194 -6.135 -5.735 0.7294 -0.6840 -0.0001

Bcc 0.2616 35.099 12.524 11.708 -0.0882 -0.0941 0.9916

Baa -0.0715 -9.600 -3.425 -3.202 -0.2362 -0.0333 0.9711

13 C(13) Bbb 0.0283 3.795 1.354 1.266 0.9444 0.2273 0.2375

Bcc 0.0433 5.805 2.071 1.936 -0.2287 0.9732 -0.0222

Baa -0.0174 -2.341 -0.835 -0.781 -0.2193 0.0080 0.9756

14 C(13) Bbb 0.0074 0.987 0.352 0.329 -0.1803 0.9824 -0.0485

Bcc 0.0101 1.354 0.483 0.452 0.9589 0.1865 0.2140

Baa -0.0174 -2.341 -0.835 -0.781 -0.2193 -0.0080 0.9756

15 C(13) Bbb 0.0074 0.987 0.352 0.329 0.1803 0.9824 0.0485

Bcc 0.0101 1.354 0.483 0.452 0.9589 -0.1865 0.2140

Baa -0.0715 -9.600 -3.425 -3.202 -0.2362 0.0333 0.9711

16 C(13) Bbb 0.0283 3.795 1.354 1.266 0.9444 -0.2273 0.2375

Bcc 0.0433 5.805 2.071 1.936 0.2287 0.9732 0.0222

Baa -0.1712 -6.602 -2.356 -2.202 0.9652 -0.0000 0.2616

17 N(14) Bbb -0.1638 -6.318 -2.254 -2.107 0.0000 1.0000 0.0000

Bcc 0.3350 12.919 4.610 4.309 -0.2616 -0.0000 0.9652

Baa -0.1334 -17.906 -6.389 -5.973 -0.6783 0.7233 -0.1290

18 C(13) Bbb -0.1281 -17.194 -6.135 -5.735 0.7294 0.6840 -0.0001

Bcc 0.2616 35.099 12.524 11.708 -0.0882 0.0941 0.9916

Baa -0.0363 -4.872 -1.739 -1.625 0.0102 0.2065 0.9784

19 C(13) Bbb 0.0123 1.648 0.588 0.550 0.1084 0.9725 -0.2064

Bcc 0.0240 3.224 1.150 1.075 0.9941 -0.1081 0.0124

Baa -0.0053 -0.705 -0.251 -0.235 0.2992 0.7487 -0.5916

20 C(13) Bbb -0.0029 -0.395 -0.141 -0.132 0.9493 -0.1706 0.2642

Bcc 0.0082 1.100 0.392 0.367 -0.0969 0.6406 0.7617

Baa -0.0053 -0.705 -0.251 -0.235 -0.2992 0.7487 -0.5916

21 C(13) Bbb -0.0029 -0.395 -0.141 -0.132 0.9493 0.1706 -0.2642

Bcc 0.0082 1.100 0.392 0.367 0.0969 0.6406 0.7617

Baa -0.0363 -4.872 -1.739 -1.625 -0.0102 0.2065 0.9784

22 C(13) Bbb 0.0123 1.648 0.588 0.550 -0.1084 0.9725 -0.2064

Bcc 0.0240 3.224 1.150 1.075 0.9941 0.1081 -0.0124

Baa -0.0797 -3.075 -1.097 -1.026 0.0000 0.9453 -0.3263

23 N(14) Bbb -0.0727 -2.805 -1.001 -0.935 1.0000 -0.0000 0.0000

Bcc 0.1524 5.879 2.098 1.961 -0.0000 0.3263 0.9453

Baa -0.1334 -17.906 -6.389 -5.973 0.6783 0.7233 -0.1290

24 C(13) Bbb -0.1281 -17.194 -6.135 -5.735 0.7294 -0.6840 0.0001

Bcc 0.2616 35.099 12.524 11.708 0.0882 0.0941 0.9916

Baa -0.0135 -1.818 -0.649 -0.606 0.6467 -0.6354 -0.4219

25 C(13) Bbb 0.0058 0.785 0.280 0.262 0.6064 0.7639 -0.2208

Bcc 0.0077 1.034 0.369 0.345 0.4626 -0.1130 0.8793

Baa -0.0157 -2.102 -0.750 -0.701 0.7349 0.0203 0.6779

26 C(13) Bbb -0.0111 -1.495 -0.533 -0.499 -0.5694 -0.5244 0.6330

Bcc 0.0268 3.597 1.283 1.200 -0.3684 0.8512 0.3739

Baa -0.0116 -1.558 -0.556 -0.520 -0.5635 0.4691 0.6800

27 C(13) Bbb 0.0040 0.536 0.191 0.179 0.5509 -0.4001 0.7325

Bcc 0.0076 1.022 0.365 0.341 0.6156 0.7874 -0.0330

Baa -0.0152 -2.037 -0.727 -0.679 0.4729 -0.4910 0.7316

28 C(13) Bbb -0.0128 -1.718 -0.613 -0.573 0.7100 0.7041 0.0136

Bcc 0.0280 3.755 1.340 1.253 -0.5218 0.5130 0.6816

Baa -0.0114 -1.530 -0.546 -0.510 -0.4547 0.5681 0.6859

29 C(13) Bbb 0.0038 0.509 0.181 0.170 0.3774 -0.5747 0.7261

Bcc 0.0076 1.021 0.364 0.341 0.8067 0.5891 0.0469

Baa -0.0155 -2.074 -0.740 -0.692 0.0470 0.7699 -0.6364

30 C(13) Bbb -0.0112 -1.501 -0.536 -0.501 0.4938 0.5359 0.6848

Bcc 0.0266 3.575 1.276 1.192 0.8683 -0.3465 -0.3550

Baa -0.0152 -2.037 -0.727 -0.679 -0.4729 -0.4910 0.7316

31 C(13) Bbb -0.0128 -1.718 -0.613 -0.573 0.7100 -0.7041 -0.0136

Bcc 0.0280 3.755 1.340 1.253 0.5218 0.5130 0.6816

Baa -0.0116 -1.558 -0.556 -0.520 0.5635 0.4691 0.6800

32 C(13) Bbb 0.0040 0.536 0.191 0.179 -0.5509 -0.4001 0.7325

Bcc 0.0076 1.022 0.365 0.341 -0.6156 0.7874 -0.0330

Baa -0.0157 -2.102 -0.750 -0.701 0.7349 -0.0203 -0.6779

33 C(13) Bbb -0.0111 -1.495 -0.533 -0.499 0.5694 -0.5244 0.6330

Bcc 0.0268 3.597 1.283 1.200 0.3684 0.8512 0.3739

Baa -0.0135 -1.818 -0.649 -0.606 0.6467 0.6354 0.4219

34 C(13) Bbb 0.0058 0.785 0.280 0.262 -0.6064 0.7639 -0.2208

Bcc 0.0077 1.034 0.369 0.345 -0.4626 -0.1130 0.8793

Baa -0.0155 -2.074 -0.740 -0.692 -0.0470 0.7699 -0.6364

35 C(13) Bbb -0.0112 -1.501 -0.536 -0.501 -0.4938 0.5359 0.6848

Bcc 0.0266 3.575 1.276 1.192 0.8683 0.3465 0.3550

Baa -0.0114 -1.530 -0.546 -0.510 0.4547 0.5681 0.6859

36 C(13) Bbb 0.0038 0.509 0.181 0.170 -0.3774 -0.5747 0.7261

Bcc 0.0076 1.021 0.364 0.341 0.8067 -0.5891 -0.0469

Baa -0.0135 -1.818 -0.649 -0.606 0.6467 0.6354 -0.4219

37 C(13) Bbb 0.0058 0.785 0.280 0.262 -0.6064 0.7639 0.2208

Bcc 0.0077 1.034 0.369 0.345 0.4626 0.1130 0.8793

Baa -0.0155 -2.074 -0.740 -0.692 -0.0470 0.7699 0.6364

38 C(13) Bbb -0.0112 -1.501 -0.536 -0.501 0.4938 -0.5359 0.6848

Bcc 0.0266 3.575 1.276 1.192 0.8683 0.3465 -0.3550

Baa -0.0114 -1.530 -0.546 -0.510 -0.4547 -0.5681 0.6859

39 C(13) Bbb 0.0038 0.509 0.181 0.170 0.3774 0.5747 0.7261

Bcc 0.0076 1.021 0.364 0.341 0.8067 -0.5891 0.0469

Baa -0.0152 -2.037 -0.727 -0.679 0.4729 0.4910 0.7316

40 C(13) Bbb -0.0128 -1.718 -0.613 -0.573 0.7100 -0.7041 0.0136

Bcc 0.0280 3.755 1.340 1.253 -0.5218 -0.5130 0.6816

Baa -0.0116 -1.558 -0.556 -0.520 -0.5635 -0.4691 0.6800

41 C(13) Bbb 0.0040 0.536 0.191 0.179 0.5509 0.4001 0.7325

Bcc 0.0076 1.022 0.365 0.341 -0.6156 0.7874 0.0330

Baa -0.0157 -2.102 -0.750 -0.701 0.7349 -0.0203 0.6779

42 C(13) Bbb -0.0111 -1.495 -0.533 -0.499 -0.5694 0.5244 0.6330

Bcc 0.0268 3.597 1.283 1.200 0.3684 0.8512 -0.3739

Baa -0.0135 -1.818 -0.649 -0.606 0.6467 -0.6354 0.4219

43 C(13) Bbb 0.0058 0.785 0.280 0.262 0.6064 0.7639 0.2208

Bcc 0.0077 1.034 0.369 0.345 -0.4626 0.1130 0.8793

Baa -0.0155 -2.074 -0.740 -0.692 0.0470 0.7699 0.6364

44 C(13) Bbb -0.0112 -1.501 -0.536 -0.501 -0.4938 -0.5359 0.6848

Bcc 0.0266 3.575 1.276 1.192 0.8683 -0.3465 0.3550

Baa -0.0114 -1.530 -0.546 -0.510 0.4547 -0.5681 0.6859

45 C(13) Bbb 0.0038 0.509 0.181 0.170 -0.3774 0.5747 0.7261

Bcc 0.0076 1.021 0.364 0.341 0.8067 0.5891 -0.0469

Baa -0.0152 -2.037 -0.727 -0.679 -0.4729 0.4910 0.7316

46 C(13) Bbb -0.0128 -1.718 -0.613 -0.573 0.7100 0.7041 -0.0136

Bcc 0.0280 3.755 1.340 1.253 0.5218 -0.5130 0.6816

Baa -0.0116 -1.558 -0.556 -0.520 0.5635 -0.4691 0.6800

47 C(13) Bbb 0.0040 0.536 0.191 0.179 -0.5509 0.4001 0.7325

Bcc 0.0076 1.022 0.365 0.341 0.6156 0.7874 0.0330

Baa -0.0157 -2.102 -0.750 -0.701 0.7349 0.0203 -0.6779

48 C(13) Bbb -0.0111 -1.495 -0.533 -0.499 0.5694 0.5244 0.6330

Bcc 0.0268 3.597 1.283 1.200 -0.3684 0.8512 -0.3739

Baa -0.0016 -0.856 -0.305 -0.286 0.0429 -0.2459 0.9683

49 H(1) Bbb 0.0004 0.233 0.083 0.078 0.9958 0.0892 -0.0214

Bcc 0.0012 0.623 0.222 0.208 -0.0811 0.9652 0.2487

Baa -0.0016 -0.856 -0.305 -0.286 -0.0429 -0.2459 0.9683

50 H(1) Bbb 0.0004 0.233 0.083 0.078 0.9958 -0.0892 0.0214

Bcc 0.0012 0.623 0.222 0.208 0.0811 0.9652 0.2487

Baa -0.0013 -0.702 -0.250 -0.234 -0.0080 0.3642 0.9313

51 H(1) Bbb -0.0009 -0.488 -0.174 -0.163 -0.6165 0.7315 -0.2913

Bcc 0.0022 1.190 0.424 0.397 0.7873 0.5765 -0.2186

Baa -0.0013 -0.702 -0.250 -0.234 -0.0080 -0.3642 0.9313

52 H(1) Bbb -0.0009 -0.488 -0.174 -0.163 0.6165 0.7315 0.2913

Bcc 0.0022 1.190 0.424 0.397 0.7873 -0.5765 -0.2186

Baa -0.0013 -0.702 -0.250 -0.234 0.0080 -0.3642 0.9313

53 H(1) Bbb -0.0009 -0.488 -0.174 -0.163 -0.6165 0.7315 0.2913

Bcc 0.0022 1.190 0.424 0.397 0.7873 0.5765 0.2186

Baa -0.0013 -0.702 -0.250 -0.234 0.0080 0.3642 0.9313

54 H(1) Bbb -0.0009 -0.488 -0.174 -0.163 0.6165 0.7315 -0.2913

Bcc 0.0022 1.190 0.424 0.397 0.7873 -0.5765 0.2186

Baa -0.0016 -0.856 -0.305 -0.286 0.0429 0.2459 0.9683

55 H(1) Bbb 0.0004 0.233 0.083 0.078 0.9958 -0.0892 -0.0214

Bcc 0.0012 0.623 0.222 0.208 0.0811 0.9652 -0.2487

Baa -0.0016 -0.856 -0.305 -0.286 -0.0429 0.2459 0.9683

56 H(1) Bbb 0.0004 0.233 0.083 0.078 0.9958 0.0892 0.0214

Bcc 0.0012 0.623 0.222 0.208 -0.0811 0.9652 -0.2487

Baa -0.0023 -1.242 -0.443 -0.414 -0.3634 0.4757 0.8010

57 H(1) Bbb -0.0002 -0.094 -0.034 -0.032 0.8618 0.4983 0.0951

Bcc 0.0025 1.336 0.477 0.446 -0.3539 0.7249 -0.5910

Baa -0.0008 -0.401 -0.143 -0.134 0.5899 -0.5679 -0.5741

58 H(1) Bbb -0.0001 -0.056 -0.020 -0.019 0.4149 -0.3968 0.8188

Bcc 0.0009 0.457 0.163 0.153 0.6928 0.7212 -0.0015

Baa -0.0020 -1.094 -0.390 -0.365 0.4468 -0.4572 0.7689

59 H(1) Bbb -0.0005 -0.244 -0.087 -0.081 -0.5413 0.5461 0.6393

Bcc 0.0025 1.338 0.477 0.446 0.7123 0.7019 0.0035

Baa -0.0008 -0.406 -0.145 -0.136 -0.5338 0.6078 0.5879

60 H(1) Bbb -0.0000 -0.023 -0.008 -0.008 0.3819 -0.4471 0.8089

Bcc 0.0008 0.430 0.153 0.143 0.7545 0.6563 0.0066

Baa -0.0025 -1.316 -0.470 -0.439 -0.4028 0.4244 0.8110

61 H(1) Bbb -0.0002 -0.125 -0.044 -0.042 0.5779 0.8050 -0.1343

Bcc 0.0027 1.441 0.514 0.481 0.7098 -0.4145 0.5695

Baa -0.0020 -1.094 -0.390 -0.365 -0.4468 -0.4572 0.7689

62 H(1) Bbb -0.0005 -0.244 -0.087 -0.081 0.5413 0.5461 0.6393

Bcc 0.0025 1.338 0.477 0.446 0.7123 -0.7019 -0.0035

Baa -0.0008 -0.401 -0.143 -0.134 0.5899 0.5679 0.5741

63 H(1) Bbb -0.0001 -0.056 -0.020 -0.019 -0.4149 -0.3968 0.8188

Bcc 0.0009 0.457 0.163 0.153 -0.6928 0.7212 -0.0015

Baa -0.0023 -1.242 -0.443 -0.414 0.3634 0.4757 0.8010

64 H(1) Bbb -0.0002 -0.094 -0.034 -0.032 0.8618 -0.4983 -0.0951

Bcc 0.0025 1.336 0.477 0.446 0.3539 0.7249 -0.5910

Baa -0.0025 -1.316 -0.470 -0.439 0.4028 0.4244 0.8110

65 H(1) Bbb -0.0002 -0.125 -0.044 -0.042 -0.5779 0.8050 -0.1343

Bcc 0.0027 1.441 0.514 0.481 0.7098 0.4145 -0.5695

Baa -0.0008 -0.406 -0.145 -0.136 0.5338 0.6078 0.5879

66 H(1) Bbb -0.0000 -0.023 -0.008 -0.008 -0.3819 -0.4471 0.8089

Bcc 0.0008 0.430 0.153 0.143 0.7545 -0.6563 -0.0066

Baa -0.0025 -1.316 -0.470 -0.439 -0.4028 -0.4244 0.8110

67 H(1) Bbb -0.0002 -0.125 -0.044 -0.042 -0.5779 0.8050 0.1343

Bcc 0.0027 1.441 0.514 0.481 0.7098 0.4145 0.5695

Baa -0.0008 -0.406 -0.145 -0.136 0.5338 0.6078 -0.5879

68 H(1) Bbb -0.0000 -0.023 -0.008 -0.008 0.3819 0.4471 0.8089

Bcc 0.0008 0.430 0.153 0.143 0.7545 -0.6563 0.0066

Baa -0.0020 -1.094 -0.390 -0.365 0.4468 0.4572 0.7689

69 H(1) Bbb -0.0005 -0.244 -0.087 -0.081 -0.5413 -0.5461 0.6393

Bcc 0.0025 1.338 0.477 0.446 0.7123 -0.7019 0.0035

Baa -0.0008 -0.401 -0.143 -0.134 0.5899 0.5679 -0.5741

70 H(1) Bbb -0.0001 -0.056 -0.020 -0.019 0.4149 0.3968 0.8188

Bcc 0.0009 0.457 0.163 0.153 -0.6928 0.7212 0.0015

Baa -0.0023 -1.242 -0.443 -0.414 -0.3634 -0.4757 0.8010

71 H(1) Bbb -0.0002 -0.094 -0.034 -0.032 0.8618 -0.4983 0.0951

Bcc 0.0025 1.336 0.477 0.446 0.3539 0.7249 0.5910

Baa -0.0025 -1.316 -0.470 -0.439 0.4028 -0.4244 0.8110

72 H(1) Bbb -0.0002 -0.125 -0.044 -0.042 0.5779 0.8050 0.1343

Bcc 0.0027 1.441 0.514 0.481 0.7098 -0.4145 -0.5695

Baa -0.0008 -0.406 -0.145 -0.136 -0.5338 0.6078 -0.5879

73 H(1) Bbb -0.0000 -0.023 -0.008 -0.008 -0.3819 0.4471 0.8089

Bcc 0.0008 0.430 0.153 0.143 0.7545 0.6563 -0.0066

Baa -0.0020 -1.094 -0.390 -0.365 -0.4468 0.4572 0.7689

74 H(1) Bbb -0.0005 -0.244 -0.087 -0.081 0.5413 -0.5461 0.6393

Bcc 0.0025 1.338 0.477 0.446 0.7123 0.7019 -0.0035

Baa -0.0008 -0.401 -0.143 -0.134 0.5899 -0.5679 0.5741

75 H(1) Bbb -0.0001 -0.056 -0.020 -0.019 -0.4149 0.3968 0.8188

Bcc 0.0009 0.457 0.163 0.153 0.6928 0.7212 0.0015

Baa -0.0023 -1.242 -0.443 -0.414 0.3634 -0.4757 0.8010

76 H(1) Bbb -0.0002 -0.094 -0.034 -0.032 0.8618 0.4983 -0.0951

Bcc 0.0025 1.336 0.477 0.446 -0.3539 0.7249 0.5910

Baa -0.0058 -3.085 -1.101 -1.029 -0.0000 -0.2477 0.9688

77 H(1) Bbb -0.0015 -0.797 -0.284 -0.266 1.0000 0.0000 0.0000

Bcc 0.0073 3.882 1.385 1.295 -0.0000 0.9688 0.2477

Baa -0.0058 -3.085 -1.101 -1.029 -0.0000 0.2477 0.9688

78 H(1) Bbb -0.0015 -0.797 -0.284 -0.266 1.0000 -0.0000 0.0000

Bcc 0.0073 3.882 1.385 1.295 0.0000 0.9688 -0.2477

---------------------------------------------------------------------------------

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Sun Aug 18 14:40:32 2019, MaxMem= 2013265920 cpu: 36.5

(Enter /home/kira/g09/l9999.exe)

1\1\ WCSS.PL-BEM-DHCP-129-94-99-158\FOpt\UB3LYP\6-311G(d)\C44H30N4(1+,

2)\KIRA\18-Aug-2019\0\\#p opt b3lyp/6-311G\* scrf=(solvent=dmso,smd) em

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93\C,-4.2115491533,0.6779526272,-0.5300183663\C,-4.2115491533,-0.67795

26272,-0.5300183663\C,-2.8607275904,-1.087658756,-0.1765198793\N,-2.05

29968564,0.,-0.0021639229\C,-2.4606429712,-2.4303151361,-0.0101564015\

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76,0.,0.,0.\PG=C02V [SGV(H2N2),SGV'(N2),X(C44H28)]\\@

SCIENCE AND PEACE WILL TRIUMPH OVER IGNORANCE AND WAR

-- PASTEUR

Job cpu time: 0 days 7 hours 52 minutes 24.8 seconds.

File lengths (MBytes): RWF= 1955 Int= 0 D2E= 0 Chk= 87 Scr= 1

Normal termination of Gaussian 09 at Sun Aug 18 14:40:32 2019.