Entering Gaussian System, Link 0=g09

Input=ZntAzPanion.com

Output=ZntAzPanion.log

Initial command:

/home/blab/g09/l1.exe "/home/blab/g09/scratch/Gau-26972.inp" -scrdir="/home/blab/g09/scratch/"

Entering Link 1 = /home/blab/g09/l1.exe PID= 26979.

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Cite this work as:

Gaussian 09, Revision E.01,

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

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

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

17-Sep-2019

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

%nprocshared=18

Will use up to 18 processors via shared memory.

%mem=18GB

%chk=ZntAzPanion.chk

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

#p opt=GDIIS b3lyp/genecp scrf=(solvent=dmso,smd) empiricaldispersion=

gd3bj

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

Warning! Use of Opt=GDIIS is deprecated since it is seldom a good choice.

1/14=-1,18=20,19=11,26=3,38=1/1,3;

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

3/5=7,11=2,16=1,17=8,25=1,30=1,70=32201,71=1,72=21,74=-5,124=41/1,2,3;

4//1;

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

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

7//1,2,3,16;

1/14=-1,18=20,19=11,26=3/3(2);

2/9=110/2;

99//99;

2/9=110/2;

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

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

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

7//1,2,3,16;

1/14=-1,18=20,19=11,26=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 Tue Sep 17 13:48:11 2019, MaxMem= 2415919104 cpu: 1.1

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

-----------

ZntAzPanion

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Symbolic Z-matrix:

Charge = -1 Multiplicity = 2

C -2.06677 -2.19041 0.

N -0.7423 -1.86521 0.

C 0. -3.00728 0.

C -0.9161 -4.16652 0.

C -2.18334 -3.64784 0.

N 1.33695 -3.10409 0.

C 2.19041 -2.06677 0.

N 1.86521 -0.7423 0.

C 3.00728 0. 0.

C 4.16652 -0.9161 0.

C 3.64784 -2.18334 0.

N -3.10409 -1.33695 0.

C -4.16652 0.9161 0.

C -3.64784 2.18334 0.

C -2.19041 2.06677 0.

N -1.86521 0.7423 0.

C -3.00728 0. 0.

N -1.33695 3.10409 0.

N 0.7423 1.86521 0.

C 0. 3.00728 0.

C 0.9161 4.16652 0.

C 2.18334 3.64784 0.

C 2.06677 2.19041 0.

N 3.10409 1.33695 0.

Zn 0. 0. 0.

C -0.48237 -5.59359 0.

H -3.11869 -4.19296 0.

C 5.59359 -0.48237 0.

H 4.19296 -3.11869 0.

C -5.59359 0.48237 0.

H -4.19296 3.11869 0.

C 0.48237 5.59359 0.

H 3.11869 4.19296 0.

H -1.34628 -6.26359 0.

H 0.1302 -5.81848 0.88508

H 0.1302 -5.81848 -0.88508

H 5.81848 0.1302 0.88508

H 5.81848 0.1302 -0.88508

H 6.26359 -1.34628 0.

H -5.81848 -0.1302 0.88508

H -5.81848 -0.1302 -0.88508

H -6.26359 1.34628 0.

H -0.1302 5.81848 0.88508

H -0.1302 5.81848 -0.88508

H 1.34628 6.26359 0.

NAtoms= 45 NQM= 45 NQMF= 0 NMMI= 0 NMMIF= 0

NMic= 0 NMicF= 0.

Isotopes and Nuclear Properties:

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

in nuclear magnetons)

Atom 1 2 3 4 5 6 7 8 9 10

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

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

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

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

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

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

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

Atom 11 12 13 14 15 16 17 18 19 20

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

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

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

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

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

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

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

Atom 21 22 23 24 25 26 27 28 29 30

IAtWgt= 12 12 12 14 64 12 1 12 1 12

AtmWgt= 12.0000000 12.0000000 12.0000000 14.0030740 63.9291454 12.0000000 1.0078250 12.0000000 1.0078250 12.0000000

NucSpn= 0 0 0 2 0 0 1 0 1 0

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

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

NMagM= 0.0000000 0.0000000 0.0000000 0.4037610 0.0000000 0.0000000 2.7928460 0.0000000 2.7928460 0.0000000

AtZNuc= 6.0000000 6.0000000 6.0000000 7.0000000 30.0000000 6.0000000 1.0000000 6.0000000 1.0000000 6.0000000

Atom 31 32 33 34 35 36 37 38 39 40

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

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

NucSpn= 1 0 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 0.0000000 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460

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

Atom 41 42 43 44 45

IAtWgt= 1 1 1 1 1

AtmWgt= 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250

NucSpn= 1 1 1 1 1

AtZEff= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NMagM= 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460

AtZNuc= 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000

Leave Link 101 at Tue Sep 17 13:48:12 2019, MaxMem= 2415919104 cpu: 5.4

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Initialization pass.

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

! Initial Parameters !

! (Angstroms and Degrees) !

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

! Name Definition Value Derivative Info. !

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

! R1 R(1,2) 1.3638 estimate D2E/DX2 !

! R2 R(1,5) 1.4621 estimate D2E/DX2 !

! R3 R(1,12) 1.3433 estimate D2E/DX2 !

! R4 R(2,3) 1.3621 estimate D2E/DX2 !

! R5 R(2,25) 2.0075 estimate D2E/DX2 !

! R6 R(3,4) 1.4775 estimate D2E/DX2 !

! R7 R(3,6) 1.3404 estimate D2E/DX2 !

! R8 R(4,5) 1.3693 estimate D2E/DX2 !

! R9 R(4,26) 1.4915 estimate D2E/DX2 !

! R10 R(5,27) 1.0826 estimate D2E/DX2 !

! R11 R(6,7) 1.3433 estimate D2E/DX2 !

! R12 R(7,8) 1.3638 estimate D2E/DX2 !

! R13 R(7,11) 1.4621 estimate D2E/DX2 !

! R14 R(8,9) 1.3621 estimate D2E/DX2 !

! R15 R(8,25) 2.0075 estimate D2E/DX2 !

! R16 R(9,10) 1.4775 estimate D2E/DX2 !

! R17 R(9,24) 1.3404 estimate D2E/DX2 !

! R18 R(10,11) 1.3693 estimate D2E/DX2 !

! R19 R(10,28) 1.4915 estimate D2E/DX2 !

! R20 R(11,29) 1.0826 estimate D2E/DX2 !

! R21 R(12,17) 1.3404 estimate D2E/DX2 !

! R22 R(13,14) 1.3693 estimate D2E/DX2 !

! R23 R(13,17) 1.4775 estimate D2E/DX2 !

! R24 R(13,30) 1.4915 estimate D2E/DX2 !

! R25 R(14,15) 1.4621 estimate D2E/DX2 !

! R26 R(14,31) 1.0826 estimate D2E/DX2 !

! R27 R(15,16) 1.3638 estimate D2E/DX2 !

! R28 R(15,18) 1.3433 estimate D2E/DX2 !

! R29 R(16,17) 1.3621 estimate D2E/DX2 !

! R30 R(16,25) 2.0075 estimate D2E/DX2 !

! R31 R(18,20) 1.3404 estimate D2E/DX2 !

! R32 R(19,20) 1.3621 estimate D2E/DX2 !

! R33 R(19,23) 1.3638 estimate D2E/DX2 !

! R34 R(19,25) 2.0075 estimate D2E/DX2 !

! R35 R(20,21) 1.4775 estimate D2E/DX2 !

! R36 R(21,22) 1.3693 estimate D2E/DX2 !

! R37 R(21,32) 1.4915 estimate D2E/DX2 !

! R38 R(22,23) 1.4621 estimate D2E/DX2 !

! R39 R(22,33) 1.0826 estimate D2E/DX2 !

! R40 R(23,24) 1.3433 estimate D2E/DX2 !

! R41 R(26,34) 1.0933 estimate D2E/DX2 !

! R42 R(26,35) 1.0996 estimate D2E/DX2 !

! R43 R(26,36) 1.0996 estimate D2E/DX2 !

! R44 R(28,37) 1.0996 estimate D2E/DX2 !

! R45 R(28,38) 1.0996 estimate D2E/DX2 !

! R46 R(28,39) 1.0933 estimate D2E/DX2 !

! R47 R(30,40) 1.0996 estimate D2E/DX2 !

! R48 R(30,41) 1.0996 estimate D2E/DX2 !

! R49 R(30,42) 1.0933 estimate D2E/DX2 !

! R50 R(32,43) 1.0996 estimate D2E/DX2 !

! R51 R(32,44) 1.0996 estimate D2E/DX2 !

! R52 R(32,45) 1.0933 estimate D2E/DX2 !

! A1 A(2,1,5) 108.3677 estimate D2E/DX2 !

! A2 A(2,1,12) 126.7588 estimate D2E/DX2 !

! A3 A(5,1,12) 124.8735 estimate D2E/DX2 !

! A4 A(1,2,3) 109.2275 estimate D2E/DX2 !

! A5 A(1,2,25) 125.496 estimate D2E/DX2 !

! A6 A(3,2,25) 125.2764 estimate D2E/DX2 !

! A7 A(2,3,4) 108.6597 estimate D2E/DX2 !

! A8 A(2,3,6) 127.1639 estimate D2E/DX2 !

! A9 A(4,3,6) 124.1764 estimate D2E/DX2 !

! A10 A(3,4,5) 106.0588 estimate D2E/DX2 !

! A11 A(3,4,26) 124.7765 estimate D2E/DX2 !

! A12 A(5,4,26) 129.1647 estimate D2E/DX2 !

! A13 A(1,5,4) 107.6862 estimate D2E/DX2 !

! A14 A(1,5,27) 124.8063 estimate D2E/DX2 !

! A15 A(4,5,27) 127.5074 estimate D2E/DX2 !

! A16 A(3,6,7) 125.3048 estimate D2E/DX2 !

! A17 A(6,7,8) 126.7588 estimate D2E/DX2 !

! A18 A(6,7,11) 124.8735 estimate D2E/DX2 !

! A19 A(8,7,11) 108.3677 estimate D2E/DX2 !

! A20 A(7,8,9) 109.2275 estimate D2E/DX2 !

! A21 A(7,8,25) 125.496 estimate D2E/DX2 !

! A22 A(9,8,25) 125.2764 estimate D2E/DX2 !

! A23 A(8,9,10) 108.6597 estimate D2E/DX2 !

! A24 A(8,9,24) 127.1639 estimate D2E/DX2 !

! A25 A(10,9,24) 124.1764 estimate D2E/DX2 !

! A26 A(9,10,11) 106.0588 estimate D2E/DX2 !

! A27 A(9,10,28) 124.7765 estimate D2E/DX2 !

! A28 A(11,10,28) 129.1647 estimate D2E/DX2 !

! A29 A(7,11,10) 107.6862 estimate D2E/DX2 !

! A30 A(7,11,29) 124.8063 estimate D2E/DX2 !

! A31 A(10,11,29) 127.5074 estimate D2E/DX2 !

! A32 A(1,12,17) 125.3048 estimate D2E/DX2 !

! A33 A(14,13,17) 106.0588 estimate D2E/DX2 !

! A34 A(14,13,30) 129.1647 estimate D2E/DX2 !

! A35 A(17,13,30) 124.7765 estimate D2E/DX2 !

! A36 A(13,14,15) 107.6862 estimate D2E/DX2 !

! A37 A(13,14,31) 127.5074 estimate D2E/DX2 !

! A38 A(15,14,31) 124.8063 estimate D2E/DX2 !

! A39 A(14,15,16) 108.3677 estimate D2E/DX2 !

! A40 A(14,15,18) 124.8735 estimate D2E/DX2 !

! A41 A(16,15,18) 126.7588 estimate D2E/DX2 !

! A42 A(15,16,17) 109.2275 estimate D2E/DX2 !

! A43 A(15,16,25) 125.496 estimate D2E/DX2 !

! A44 A(17,16,25) 125.2764 estimate D2E/DX2 !

! A45 A(12,17,13) 124.1764 estimate D2E/DX2 !

! A46 A(12,17,16) 127.1639 estimate D2E/DX2 !

! A47 A(13,17,16) 108.6597 estimate D2E/DX2 !

! A48 A(15,18,20) 125.3048 estimate D2E/DX2 !

! A49 A(20,19,23) 109.2275 estimate D2E/DX2 !

! A50 A(20,19,25) 125.2764 estimate D2E/DX2 !

! A51 A(23,19,25) 125.496 estimate D2E/DX2 !

! A52 A(18,20,19) 127.1639 estimate D2E/DX2 !

! A53 A(18,20,21) 124.1764 estimate D2E/DX2 !

! A54 A(19,20,21) 108.6597 estimate D2E/DX2 !

! A55 A(20,21,22) 106.0588 estimate D2E/DX2 !

! A56 A(20,21,32) 124.7765 estimate D2E/DX2 !

! A57 A(22,21,32) 129.1647 estimate D2E/DX2 !

! A58 A(21,22,23) 107.6862 estimate D2E/DX2 !

! A59 A(21,22,33) 127.5074 estimate D2E/DX2 !

! A60 A(23,22,33) 124.8063 estimate D2E/DX2 !

! A61 A(19,23,22) 108.3677 estimate D2E/DX2 !

! A62 A(19,23,24) 126.7588 estimate D2E/DX2 !

! A63 A(22,23,24) 124.8735 estimate D2E/DX2 !

! A64 A(9,24,23) 125.3048 estimate D2E/DX2 !

! A65 A(2,25,8) 90.0 estimate D2E/DX2 !

! A66 A(2,25,16) 90.0 estimate D2E/DX2 !

! A67 A(8,25,19) 90.0 estimate D2E/DX2 !

! A68 A(16,25,19) 90.0 estimate D2E/DX2 !

! A69 A(4,26,34) 110.889 estimate D2E/DX2 !

! A70 A(4,26,35) 110.9568 estimate D2E/DX2 !

! A71 A(4,26,36) 110.9568 estimate D2E/DX2 !

! A72 A(34,26,35) 108.353 estimate D2E/DX2 !

! A73 A(34,26,36) 108.353 estimate D2E/DX2 !

! A74 A(35,26,36) 107.1998 estimate D2E/DX2 !

! A75 A(10,28,37) 110.9568 estimate D2E/DX2 !

! A76 A(10,28,38) 110.9568 estimate D2E/DX2 !

! A77 A(10,28,39) 110.889 estimate D2E/DX2 !

! A78 A(37,28,38) 107.1998 estimate D2E/DX2 !

! A79 A(37,28,39) 108.353 estimate D2E/DX2 !

! A80 A(38,28,39) 108.353 estimate D2E/DX2 !

! A81 A(13,30,40) 110.9568 estimate D2E/DX2 !

! A82 A(13,30,41) 110.9568 estimate D2E/DX2 !

! A83 A(13,30,42) 110.889 estimate D2E/DX2 !

! A84 A(40,30,41) 107.1998 estimate D2E/DX2 !

! A85 A(40,30,42) 108.353 estimate D2E/DX2 !

! A86 A(41,30,42) 108.353 estimate D2E/DX2 !

! A87 A(21,32,43) 110.9568 estimate D2E/DX2 !

! A88 A(21,32,44) 110.9568 estimate D2E/DX2 !

! A89 A(21,32,45) 110.889 estimate D2E/DX2 !

! A90 A(43,32,44) 107.1998 estimate D2E/DX2 !

! A91 A(43,32,45) 108.353 estimate D2E/DX2 !

! A92 A(44,32,45) 108.353 estimate D2E/DX2 !

! A93 L(2,25,19,16,-1) 180.0 estimate D2E/DX2 !

! A94 L(8,25,16,19,-1) 180.0 estimate D2E/DX2 !

! A95 L(2,25,19,16,-2) 180.0 estimate D2E/DX2 !

! A96 L(8,25,16,19,-2) 180.0 estimate D2E/DX2 !

! D1 D(5,1,2,3) 0.0 estimate D2E/DX2 !

! D2 D(5,1,2,25) 180.0 estimate D2E/DX2 !

! D3 D(12,1,2,3) 180.0 estimate D2E/DX2 !

! D4 D(12,1,2,25) 0.0 estimate D2E/DX2 !

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

! D6 D(2,1,5,27) 180.0 estimate D2E/DX2 !

! D7 D(12,1,5,4) 180.0 estimate D2E/DX2 !

! D8 D(12,1,5,27) 0.0 estimate D2E/DX2 !

! D9 D(2,1,12,17) 0.0 estimate D2E/DX2 !

! D10 D(5,1,12,17) 180.0 estimate D2E/DX2 !

! D11 D(1,2,3,4) 0.0 estimate D2E/DX2 !

! D12 D(1,2,3,6) 180.0 estimate D2E/DX2 !

! D13 D(25,2,3,4) 180.0 estimate D2E/DX2 !

! D14 D(25,2,3,6) 0.0 estimate D2E/DX2 !

! D15 D(1,2,25,8) 180.0 estimate D2E/DX2 !

! D16 D(1,2,25,16) 0.0 estimate D2E/DX2 !

! D17 D(3,2,25,8) 0.0 estimate D2E/DX2 !

! D18 D(3,2,25,16) 180.0 estimate D2E/DX2 !

! D19 D(2,3,4,5) 0.0 estimate D2E/DX2 !

! D20 D(2,3,4,26) 180.0 estimate D2E/DX2 !

! D21 D(6,3,4,5) 180.0 estimate D2E/DX2 !

! D22 D(6,3,4,26) 0.0 estimate D2E/DX2 !

! D23 D(2,3,6,7) 0.0 estimate D2E/DX2 !

! D24 D(4,3,6,7) 180.0 estimate D2E/DX2 !

! D25 D(3,4,5,1) 0.0 estimate D2E/DX2 !

! D26 D(3,4,5,27) 180.0 estimate D2E/DX2 !

! D27 D(26,4,5,1) 180.0 estimate D2E/DX2 !

! D28 D(26,4,5,27) 0.0 estimate D2E/DX2 !

! D29 D(3,4,26,34) 180.0 estimate D2E/DX2 !

! D30 D(3,4,26,35) 59.5315 estimate D2E/DX2 !

! D31 D(3,4,26,36) -59.5315 estimate D2E/DX2 !

! D32 D(5,4,26,34) 0.0 estimate D2E/DX2 !

! D33 D(5,4,26,35) -120.4685 estimate D2E/DX2 !

! D34 D(5,4,26,36) 120.4685 estimate D2E/DX2 !

! D35 D(3,6,7,8) 0.0 estimate D2E/DX2 !

! D36 D(3,6,7,11) 180.0 estimate D2E/DX2 !

! D37 D(6,7,8,9) 180.0 estimate D2E/DX2 !

! D38 D(6,7,8,25) 0.0 estimate D2E/DX2 !

! D39 D(11,7,8,9) 0.0 estimate D2E/DX2 !

! D40 D(11,7,8,25) 180.0 estimate D2E/DX2 !

! D41 D(6,7,11,10) 180.0 estimate D2E/DX2 !

! D42 D(6,7,11,29) 0.0 estimate D2E/DX2 !

! D43 D(8,7,11,10) 0.0 estimate D2E/DX2 !

! D44 D(8,7,11,29) 180.0 estimate D2E/DX2 !

! D45 D(7,8,9,10) 0.0 estimate D2E/DX2 !

! D46 D(7,8,9,24) 180.0 estimate D2E/DX2 !

! D47 D(25,8,9,10) 180.0 estimate D2E/DX2 !

! D48 D(25,8,9,24) 0.0 estimate D2E/DX2 !

! D49 D(7,8,25,2) 0.0 estimate D2E/DX2 !

! D50 D(7,8,25,19) 180.0 estimate D2E/DX2 !

! D51 D(9,8,25,2) 180.0 estimate D2E/DX2 !

! D52 D(9,8,25,19) 0.0 estimate D2E/DX2 !

! D53 D(8,9,10,11) 0.0 estimate D2E/DX2 !

! D54 D(8,9,10,28) 180.0 estimate D2E/DX2 !

! D55 D(24,9,10,11) 180.0 estimate D2E/DX2 !

! D56 D(24,9,10,28) 0.0 estimate D2E/DX2 !

! D57 D(8,9,24,23) 0.0 estimate D2E/DX2 !

! D58 D(10,9,24,23) 180.0 estimate D2E/DX2 !

! D59 D(9,10,11,7) 0.0 estimate D2E/DX2 !

! D60 D(9,10,11,29) 180.0 estimate D2E/DX2 !

! D61 D(28,10,11,7) 180.0 estimate D2E/DX2 !

! D62 D(28,10,11,29) 0.0 estimate D2E/DX2 !

! D63 D(9,10,28,37) 59.5315 estimate D2E/DX2 !

! D64 D(9,10,28,38) -59.5315 estimate D2E/DX2 !

! D65 D(9,10,28,39) 180.0 estimate D2E/DX2 !

! D66 D(11,10,28,37) -120.4685 estimate D2E/DX2 !

! D67 D(11,10,28,38) 120.4685 estimate D2E/DX2 !

! D68 D(11,10,28,39) 0.0 estimate D2E/DX2 !

! D69 D(1,12,17,13) 180.0 estimate D2E/DX2 !

! D70 D(1,12,17,16) 0.0 estimate D2E/DX2 !

! D71 D(17,13,14,15) 0.0 estimate D2E/DX2 !

! D72 D(17,13,14,31) 180.0 estimate D2E/DX2 !

! D73 D(30,13,14,15) 180.0 estimate D2E/DX2 !

! D74 D(30,13,14,31) 0.0 estimate D2E/DX2 !

! D75 D(14,13,17,12) 180.0 estimate D2E/DX2 !

! D76 D(14,13,17,16) 0.0 estimate D2E/DX2 !

! D77 D(30,13,17,12) 0.0 estimate D2E/DX2 !

! D78 D(30,13,17,16) 180.0 estimate D2E/DX2 !

! D79 D(14,13,30,40) -120.4685 estimate D2E/DX2 !

! D80 D(14,13,30,41) 120.4685 estimate D2E/DX2 !

! D81 D(14,13,30,42) 0.0 estimate D2E/DX2 !

! D82 D(17,13,30,40) 59.5315 estimate D2E/DX2 !

! D83 D(17,13,30,41) -59.5315 estimate D2E/DX2 !

! D84 D(17,13,30,42) 180.0 estimate D2E/DX2 !

! D85 D(13,14,15,16) 0.0 estimate D2E/DX2 !

! D86 D(13,14,15,18) 180.0 estimate D2E/DX2 !

! D87 D(31,14,15,16) 180.0 estimate D2E/DX2 !

! D88 D(31,14,15,18) 0.0 estimate D2E/DX2 !

! D89 D(14,15,16,17) 0.0 estimate D2E/DX2 !

! D90 D(14,15,16,25) 180.0 estimate D2E/DX2 !

! D91 D(18,15,16,17) 180.0 estimate D2E/DX2 !

! D92 D(18,15,16,25) 0.0 estimate D2E/DX2 !

! D93 D(14,15,18,20) 180.0 estimate D2E/DX2 !

! D94 D(16,15,18,20) 0.0 estimate D2E/DX2 !

! D95 D(15,16,17,12) 180.0 estimate D2E/DX2 !

! D96 D(15,16,17,13) 0.0 estimate D2E/DX2 !

! D97 D(25,16,17,12) 0.0 estimate D2E/DX2 !

! D98 D(25,16,17,13) 180.0 estimate D2E/DX2 !

! D99 D(15,16,25,2) 180.0 estimate D2E/DX2 !

! D100 D(15,16,25,19) 0.0 estimate D2E/DX2 !

! D101 D(17,16,25,2) 0.0 estimate D2E/DX2 !

! D102 D(17,16,25,19) 180.0 estimate D2E/DX2 !

! D103 D(15,18,20,19) 0.0 estimate D2E/DX2 !

! D104 D(15,18,20,21) 180.0 estimate D2E/DX2 !

! D105 D(23,19,20,18) 180.0 estimate D2E/DX2 !

! D106 D(23,19,20,21) 0.0 estimate D2E/DX2 !

! D107 D(25,19,20,18) 0.0 estimate D2E/DX2 !

! D108 D(25,19,20,21) 180.0 estimate D2E/DX2 !

! D109 D(20,19,23,22) 0.0 estimate D2E/DX2 !

! D110 D(20,19,23,24) 180.0 estimate D2E/DX2 !

! D111 D(25,19,23,22) 180.0 estimate D2E/DX2 !

! D112 D(25,19,23,24) 0.0 estimate D2E/DX2 !

! D113 D(20,19,25,8) 180.0 estimate D2E/DX2 !

! D114 D(20,19,25,16) 0.0 estimate D2E/DX2 !

! D115 D(23,19,25,8) 0.0 estimate D2E/DX2 !

! D116 D(23,19,25,16) 180.0 estimate D2E/DX2 !

! D117 D(18,20,21,22) 180.0 estimate D2E/DX2 !

! D118 D(18,20,21,32) 0.0 estimate D2E/DX2 !

! D119 D(19,20,21,22) 0.0 estimate D2E/DX2 !

! D120 D(19,20,21,32) 180.0 estimate D2E/DX2 !

! D121 D(20,21,22,23) 0.0 estimate D2E/DX2 !

! D122 D(20,21,22,33) 180.0 estimate D2E/DX2 !

! D123 D(32,21,22,23) 180.0 estimate D2E/DX2 !

! D124 D(32,21,22,33) 0.0 estimate D2E/DX2 !

! D125 D(20,21,32,43) 59.5315 estimate D2E/DX2 !

! D126 D(20,21,32,44) -59.5315 estimate D2E/DX2 !

! D127 D(20,21,32,45) 180.0 estimate D2E/DX2 !

! D128 D(22,21,32,43) -120.4685 estimate D2E/DX2 !

! D129 D(22,21,32,44) 120.4685 estimate D2E/DX2 !

! D130 D(22,21,32,45) 0.0 estimate D2E/DX2 !

! D131 D(21,22,23,19) 0.0 estimate D2E/DX2 !

! D132 D(21,22,23,24) 180.0 estimate D2E/DX2 !

! D133 D(33,22,23,19) 180.0 estimate D2E/DX2 !

! D134 D(33,22,23,24) 0.0 estimate D2E/DX2 !

! D135 D(19,23,24,9) 0.0 estimate D2E/DX2 !

! D136 D(22,23,24,9) 180.0 estimate D2E/DX2 !

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

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

Number of steps in this run= 270 maximum allowed number of steps= 270.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 13:48:12 2019, MaxMem= 2415919104 cpu: 0.2

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.066774 -2.190409 0.000000

2 7 0 -0.742302 -1.865213 0.000000

3 6 0 0.000000 -3.007280 0.000000

4 6 0 -0.916097 -4.166516 0.000000

5 6 0 -2.183341 -3.647838 0.000000

6 7 0 1.336945 -3.104087 0.000000

7 6 0 2.190409 -2.066774 0.000000

8 7 0 1.865213 -0.742302 0.000000

9 6 0 3.007280 0.000000 0.000000

10 6 0 4.166516 -0.916097 0.000000

11 6 0 3.647838 -2.183341 0.000000

12 7 0 -3.104087 -1.336945 0.000000

13 6 0 -4.166516 0.916097 0.000000

14 6 0 -3.647838 2.183341 0.000000

15 6 0 -2.190409 2.066774 0.000000

16 7 0 -1.865213 0.742302 0.000000

17 6 0 -3.007280 0.000000 0.000000

18 7 0 -1.336945 3.104087 0.000000

19 7 0 0.742302 1.865213 0.000000

20 6 0 0.000000 3.007280 0.000000

21 6 0 0.916097 4.166516 0.000000

22 6 0 2.183341 3.647838 0.000000

23 6 0 2.066774 2.190409 0.000000

24 7 0 3.104087 1.336945 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.482366 -5.593592 0.000000

27 1 0 -3.118690 -4.192956 0.000000

28 6 0 5.593592 -0.482366 0.000000

29 1 0 4.192956 -3.118690 0.000000

30 6 0 -5.593592 0.482366 0.000000

31 1 0 -4.192956 3.118690 0.000000

32 6 0 0.482366 5.593592 0.000000

33 1 0 3.118690 4.192956 0.000000

34 1 0 -1.346284 -6.263586 0.000000

35 1 0 0.130195 -5.818475 0.885075

36 1 0 0.130195 -5.818475 -0.885075

37 1 0 5.818475 0.130195 0.885075

38 1 0 5.818475 0.130195 -0.885075

39 1 0 6.263586 -1.346284 0.000000

40 1 0 -5.818475 -0.130195 0.885075

41 1 0 -5.818475 -0.130195 -0.885075

42 1 0 -6.263586 1.346284 0.000000

43 1 0 -0.130195 5.818475 0.885075

44 1 0 -0.130195 5.818475 -0.885075

45 1 0 1.346284 6.263586 0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.363810 0.000000

3 C 2.222349 1.362105 0.000000

4 C 2.286713 2.307856 1.477519 0.000000

5 C 1.462083 2.292236 2.275366 1.369282 0.000000

6 N 3.524218 2.420346 1.340445 2.490974 3.562033

7 C 4.258978 2.939629 2.383788 3.749573 4.650748

8 N 4.190171 2.839025 2.934134 4.411454 4.983265

9 C 5.526655 4.187885 4.252936 5.723001 6.344231

10 C 6.362215 4.999732 4.661856 6.033090 6.912532

11 C 5.714616 4.401651 3.739732 4.976192 6.012271

12 N 1.343287 2.420144 3.524965 3.576838 2.487569

13 C 3.749573 4.411454 5.723001 6.033090 4.976192

14 C 4.650748 4.983265 6.344231 6.912532 6.012271

15 C 4.258978 4.190171 5.526655 6.362215 5.714616

16 N 2.939629 2.839025 4.187885 4.999732 4.401651

17 C 2.383788 2.934134 4.252936 4.661856 3.739732

18 N 5.344562 5.004752 6.255896 7.282773 6.804769

19 N 4.933455 4.014988 4.928712 6.255561 6.241243

20 C 5.593525 4.928712 6.014560 7.232052 7.004111

21 C 7.021967 6.255561 7.232052 8.532078 8.406583

22 C 7.221399 6.241243 7.004111 8.406583 8.502635

23 C 6.023104 4.933455 5.593525 7.021967 7.221399

24 N 6.259395 5.004850 5.339255 6.815421 7.266702

25 Zn 3.011552 2.007494 3.007280 4.266039 4.251317

26 C 3.753932 3.737429 2.630910 1.491532 2.584429

27 H 2.262017 3.326501 3.336473 2.202752 1.082604

28 C 7.848479 6.485046 6.137056 7.479907 8.396481

29 H 6.328185 5.091952 4.194436 5.215397 6.398215

30 C 4.425175 5.389447 6.592867 6.594775 5.356155

31 H 5.719019 6.061873 7.423502 7.988243 7.058644

32 C 8.190774 7.558676 8.614388 9.859787 9.618213

33 H 8.224134 7.183918 7.846631 9.282256 9.465177

34 H 4.136409 4.439649 3.523636 2.140739 2.746416

35 H 4.332770 4.144018 2.950106 2.146405 3.293550

36 H 4.332770 4.144018 2.950106 2.146405 3.293550

37 H 8.267147 6.914391 6.669465 8.037384 8.893028

38 H 8.267147 6.914391 6.669465 8.037384 8.893028

39 H 8.373019 7.025080 6.480078 7.713725 8.754869

40 H 4.370709 5.437019 6.551002 6.411595 5.135306

41 H 4.370709 5.437019 6.551002 6.411595 5.135306

42 H 5.488299 6.387354 7.627977 7.680274 6.449004

43 H 8.287094 7.758679 8.870979 10.054902 9.726759

44 H 8.287094 7.758679 8.870979 10.054902 9.726759

45 H 9.116962 8.392828 9.368107 10.672647 10.521149

6 7 8 9 10

6 N 0.000000

7 C 1.343287 0.000000

8 N 2.420144 1.363810 0.000000

9 C 3.524965 2.222349 1.362105 0.000000

10 C 3.576838 2.286713 2.307856 1.477519 0.000000

11 C 2.487569 1.462083 2.292236 2.275366 1.369282

12 N 4.779703 5.344562 5.004752 6.255896 7.282773

13 C 6.815421 7.021967 6.255561 7.232052 8.532078

14 C 7.266702 7.221399 6.241243 7.004111 8.406583

15 C 6.259395 6.023104 4.933455 5.593525 7.021967

16 N 5.004850 4.933455 4.014988 4.928712 6.255561

17 C 5.339255 5.593525 4.928712 6.014560 7.232052

18 N 6.759520 6.259395 5.004850 5.339255 6.815421

19 N 5.004752 4.190171 2.839025 2.934134 4.411454

20 C 6.255896 5.526655 4.187885 4.252936 5.723001

21 C 7.282773 6.362215 4.999732 4.661856 6.033090

22 C 6.804769 5.714616 4.401651 3.739732 4.976192

23 C 5.344562 4.258978 2.939629 2.383788 3.749573

24 N 4.779703 3.524218 2.420346 1.340445 2.490974

25 Zn 3.379760 3.011552 2.007494 3.007280 4.266039

26 C 3.083428 4.425175 5.389447 6.592867 6.594775

27 H 4.586755 5.719019 6.061873 7.423502 7.988243

28 C 4.999246 3.753932 3.737429 2.630910 1.491532

29 H 2.856048 2.262017 3.326501 3.336473 2.202752

30 C 7.803524 8.190774 7.558676 8.614388 9.859787

31 H 8.324828 8.224134 7.183918 7.846631 9.282256

32 C 8.739561 7.848479 6.485046 6.137056 7.479907

33 H 7.511421 6.328185 5.091952 4.194436 5.215397

34 H 4.145136 5.488299 6.387354 7.627977 7.680274

35 H 3.099598 4.370709 5.437019 6.551002 6.411595

36 H 3.099598 4.370709 5.437019 6.551002 6.411595

37 H 5.597147 4.332770 4.144018 2.950106 2.146405

38 H 5.597147 4.332770 4.144018 2.950106 2.146405

39 H 5.230838 4.136409 4.439649 3.523636 2.140739

40 H 7.799194 8.287094 7.758679 8.870979 10.054902

41 H 7.799194 8.287094 7.758679 8.870979 10.054902

42 H 8.807603 9.116962 8.392828 9.368107 10.672647

43 H 9.085591 8.267147 6.914391 6.669465 8.037384

44 H 9.085591 8.267147 6.914391 6.669465 8.037384

45 H 9.367678 8.373019 7.025080 6.480078 7.713725

11 12 13 14 15

11 C 0.000000

12 N 6.804769 0.000000

13 C 8.406583 2.490974 0.000000

14 C 8.502635 3.562033 1.369282 0.000000

15 C 7.221399 3.524218 2.286713 1.462083 0.000000

16 N 6.241243 2.420346 2.307856 2.292236 1.363810

17 C 7.004111 1.340445 1.477519 2.275366 2.222349

18 N 7.266702 4.779703 3.576838 2.487569 1.343287

19 N 4.983265 5.004850 4.999732 4.401651 2.939629

20 C 6.344231 5.339255 4.661856 3.739732 2.383788

21 C 6.912532 6.815421 6.033090 4.976192 3.749573

22 C 6.012271 7.266702 6.912532 6.012271 4.650748

23 C 4.650748 6.259395 6.362215 5.714616 4.258978

24 N 3.562033 6.759520 7.282773 6.804769 5.344562

25 Zn 4.251317 3.379760 4.266039 4.251317 3.011552

26 C 5.356155 4.999246 7.479907 8.396481 7.848479

27 H 7.058644 2.856048 5.215397 6.398215 6.328185

28 C 2.584429 8.739561 9.859787 9.618213 8.190774

29 H 1.082604 7.511421 9.282256 9.465177 8.224134

30 C 9.618213 3.083428 1.491532 2.584429 3.753932

31 H 9.465177 4.586755 2.202752 1.082604 2.262017

32 C 8.396481 7.803524 6.594775 5.356155 4.425175

33 H 6.398215 8.324828 7.988243 7.058644 5.719019

34 H 6.449004 5.230838 7.713725 8.754869 8.373019

35 H 5.135306 5.597147 8.037384 8.893028 8.267147

36 H 5.135306 5.597147 8.037384 8.893028 8.267147

37 H 3.293550 9.085591 10.054902 9.726759 8.287094

38 H 3.293550 9.085591 10.054902 9.726759 8.287094

39 H 2.746416 9.367678 10.672647 10.521149 9.116962

40 H 9.726759 3.099598 2.146405 3.293550 4.332770

41 H 9.726759 3.099598 2.146405 3.293550 4.332770

42 H 10.521149 4.145136 2.140739 2.746416 4.136409

43 H 8.893028 7.799194 6.411595 5.135306 4.370709

44 H 8.893028 7.799194 6.411595 5.135306 4.370709

45 H 8.754869 8.807603 7.680274 6.449004 5.488299

16 17 18 19 20

16 N 0.000000

17 C 1.362105 0.000000

18 N 2.420144 3.524965 0.000000

19 N 2.839025 4.187885 2.420346 0.000000

20 C 2.934134 4.252936 1.340445 1.362105 0.000000

21 C 4.411454 5.723001 2.490974 2.307856 1.477519

22 C 4.983265 6.344231 3.562033 2.292236 2.275366

23 C 4.190171 5.526655 3.524218 1.363810 2.222349

24 N 5.004752 6.255896 4.779703 2.420144 3.524965

25 Zn 2.007494 3.007280 3.379760 2.007494 3.007280

26 C 6.485046 6.137056 8.739561 7.558676 8.614388

27 H 5.091952 4.194436 7.511421 7.183918 7.846631

28 C 7.558676 8.614388 7.803524 5.389447 6.592867

29 H 7.183918 7.846631 8.324828 6.061873 7.423502

30 C 3.737429 2.630910 4.999246 6.485046 6.137056

31 H 3.326501 3.336473 2.856048 5.091952 4.194436

32 C 5.389447 6.592867 3.083428 3.737429 2.630910

33 H 6.061873 7.423502 4.586755 3.326501 3.336473

34 H 7.025080 6.480078 9.367678 8.392828 9.368107

35 H 6.914391 6.669465 9.085591 7.758679 8.870979

36 H 6.914391 6.669465 9.085591 7.758679 8.870979

37 H 7.758679 8.870979 7.799194 5.437019 6.551002

38 H 7.758679 8.870979 7.799194 5.437019 6.551002

39 H 8.392828 9.368107 8.807603 6.387354 7.627977

40 H 4.144018 2.950106 5.597147 6.914391 6.669465

41 H 4.144018 2.950106 5.597147 6.914391 6.669465

42 H 4.439649 3.523636 5.230838 7.025080 6.480078

43 H 5.437019 6.551002 3.099598 4.144018 2.950106

44 H 5.437019 6.551002 3.099598 4.144018 2.950106

45 H 6.387354 7.627977 4.145136 4.439649 3.523636

21 22 23 24 25

21 C 0.000000

22 C 1.369282 0.000000

23 C 2.286713 1.462083 0.000000

24 N 3.576838 2.487569 1.343287 0.000000

25 Zn 4.266039 4.251317 3.011552 3.379760 0.000000

26 C 9.859787 9.618213 8.190774 7.803524 5.614352

27 H 9.282256 9.465177 8.224134 8.324828 5.225620

28 C 6.594775 5.356155 4.425175 3.083428 5.614352

29 H 7.988243 7.058644 5.719019 4.586755 5.225620

30 C 7.479907 8.396481 7.848479 8.739561 5.614352

31 H 5.215397 6.398215 6.328185 7.511421 5.225620

32 C 1.491532 2.584429 3.753932 4.999246 5.614352

33 H 2.202752 1.082604 2.262017 2.856048 5.225620

34 H 10.672647 10.521149 9.116962 8.807603 6.406636

35 H 10.054902 9.726759 8.287094 7.799194 5.886846

36 H 10.054902 9.726759 8.287094 7.799194 5.886846

37 H 6.411595 5.135306 4.370709 3.099598 5.886846

38 H 6.411595 5.135306 4.370709 3.099598 5.886846

39 H 7.680274 6.449004 5.488299 4.145136 6.406636

40 H 8.037384 8.893028 8.267147 9.085591 5.886846

41 H 8.037384 8.893028 8.267147 9.085591 5.886846

42 H 7.713725 8.754869 8.373019 9.367678 6.406636

43 H 2.146405 3.293550 4.332770 5.597147 5.886846

44 H 2.146405 3.293550 4.332770 5.597147 5.886846

45 H 2.140739 2.746416 4.136409 5.230838 6.406636

26 27 28 29 30

26 C 0.000000

27 H 2.985295 0.000000

28 C 7.939893 9.469548 0.000000

29 H 5.289969 7.390143 2.985295 0.000000

30 C 7.939893 5.289969 11.228704 10.428045 0.000000

31 H 9.469548 7.390143 10.428045 10.451241 2.985295

32 C 11.228704 10.428045 7.939893 9.469548 7.939893

33 H 10.428045 10.451241 5.289969 7.390143 9.469548

34 H 1.093273 2.725607 9.032407 6.369737 7.971668

35 H 1.099619 3.739107 7.688051 4.957643 8.558370

36 H 1.099619 3.739107 7.688051 4.957643 8.558370

37 H 8.558370 9.967242 1.099619 3.739107 11.451753

38 H 8.558370 9.967242 1.099619 3.739107 11.451753

39 H 7.971668 9.804624 1.093273 2.725607 11.997359

40 H 7.688051 4.957643 11.451753 10.485381 1.099619

41 H 7.688051 4.957643 11.451753 10.485381 1.099619

42 H 9.032407 6.369737 11.997359 11.369928 1.093273

43 H 11.451753 10.485381 8.558370 9.967242 7.688051

44 H 11.451753 10.485381 8.558370 9.967242 7.688051

45 H 11.997359 11.369928 7.971668 9.804624 9.032407

31 32 33 34 35

31 H 0.000000

32 C 5.289969 0.000000

33 H 7.390143 2.985295 0.000000

34 H 9.804624 11.997359 11.369928 0.000000

35 H 9.967242 11.451753 10.485381 1.778053 0.000000

36 H 9.967242 11.451753 10.485381 1.778053 1.770150

37 H 10.485381 7.688051 4.957643 9.643524 8.230626

38 H 10.485381 7.688051 4.957643 9.643524 8.418826

39 H 11.369928 9.032407 6.369737 9.060352 7.642142

40 H 3.739107 8.558370 9.967242 7.642142 8.230626

41 H 3.739107 8.558370 9.967242 7.642142 8.418826

42 H 2.725607 7.971668 9.804624 9.060352 9.643524

43 H 4.957643 1.099619 3.739107 12.175320 11.639863

44 H 4.957643 1.099619 3.739107 12.175320 11.773693

45 H 6.369737 1.093273 2.725607 12.813273 12.175320

36 37 38 39 40

36 H 0.000000

37 H 8.418826 0.000000

38 H 8.230626 1.770150 0.000000

39 H 7.642142 1.778053 1.778053 0.000000

40 H 8.418826 11.639863 11.773693 12.175320 0.000000

41 H 8.230626 11.773693 11.639863 12.175320 1.770150

42 H 9.643524 12.175320 12.175320 12.813273 1.778053

43 H 11.773693 8.230626 8.418826 9.643524 8.230626

44 H 11.639863 8.418826 8.230626 9.643524 8.418826

45 H 12.175320 7.642142 7.642142 9.060352 9.643524

41 42 43 44 45

41 H 0.000000

42 H 1.778053 0.000000

43 H 8.418826 7.642142 0.000000

44 H 8.230626 7.642142 1.770150 0.000000

45 H 9.643524 9.060352 1.778053 1.778053 0.000000

Stoichiometry C20H16N8Zn(1-,2)

Framework group C4H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 20

Full point group C4H NOp 8

Largest Abelian subgroup C2H NOp 4

Largest concise Abelian subgroup C2H NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.190409 2.066774 0.000000

2 7 0 -1.865213 0.742302 0.000000

3 6 0 -3.007280 0.000000 0.000000

4 6 0 -4.166516 0.916097 0.000000

5 6 0 -3.647838 2.183341 0.000000

6 7 0 -3.104087 -1.336945 0.000000

7 6 0 -2.066774 -2.190409 0.000000

8 7 0 -0.742302 -1.865213 0.000000

9 6 0 -0.000000 -3.007280 0.000000

10 6 0 -0.916097 -4.166516 0.000000

11 6 0 -2.183341 -3.647838 0.000000

12 7 0 -1.336945 3.104087 0.000000

13 6 0 0.916097 4.166516 0.000000

14 6 0 2.183341 3.647838 0.000000

15 6 0 2.066774 2.190409 0.000000

16 7 0 0.742302 1.865213 0.000000

17 6 0 0.000000 3.007280 0.000000

18 7 0 3.104087 1.336945 0.000000

19 7 0 1.865213 -0.742302 0.000000

20 6 0 3.007280 -0.000000 0.000000

21 6 0 4.166516 -0.916097 0.000000

22 6 0 3.647838 -2.183341 0.000000

23 6 0 2.190409 -2.066774 0.000000

24 7 0 1.336945 -3.104087 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -5.593592 0.482366 0.000000

27 1 0 -4.192956 3.118690 0.000000

28 6 0 -0.482366 -5.593592 0.000000

29 1 0 -3.118690 -4.192956 0.000000

30 6 0 0.482366 5.593592 0.000000

31 1 0 3.118690 4.192956 0.000000

32 6 0 5.593592 -0.482366 0.000000

33 1 0 4.192956 -3.118690 0.000000

34 1 0 -6.263586 1.346284 0.000000

35 1 0 -5.818475 -0.130195 0.885075

36 1 0 -5.818475 -0.130195 -0.885075

37 1 0 0.130195 -5.818475 0.885075

38 1 0 0.130195 -5.818475 -0.885075

39 1 0 -1.346284 -6.263586 0.000000

40 1 0 -0.130195 5.818475 0.885075

41 1 0 -0.130195 5.818475 -0.885075

42 1 0 1.346284 6.263586 0.000000

43 1 0 5.818475 0.130195 0.885075

44 1 0 5.818475 0.130195 -0.885075

45 1 0 6.263586 -1.346284 0.000000

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

Rotational constants (GHZ): 0.1821070 0.1821070 0.0912612

Leave Link 202 at Tue Sep 17 13:48:12 2019, MaxMem= 2415919104 cpu: 0.2

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

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

Centers: 25

S 1 1.00

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

S 1 1.00

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

S 1 1.00

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

P 1 1.00

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

P 1 1.00

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

D 3 1.00

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

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

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

D 1 1.00

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

D 1 1.00

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

\*\*\*\*

Centers: 27 29 31 33 34 35 36 37 38 39

Centers: 40 41 42 43 44 45 1 3 4 5

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

Centers: 22 23 26 28 30 32 2 6 8 12

Centers: 16 18 19 24

6-311G\*

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

Pseudopotential Parameters

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

Center Atomic Valence Angular Power

Number Number Electrons Momentum of R Exponent Coefficient SO-Coeffient

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

1 6

No pseudopotential on this center.

2 7

No pseudopotential on this center.

3 6

No pseudopotential on this center.

4 6

No pseudopotential on this center.

5 6

No pseudopotential on this center.

6 7

No pseudopotential on this center.

7 6

No pseudopotential on this center.

8 7

No pseudopotential on this center.

9 6

No pseudopotential on this center.

10 6

No pseudopotential on this center.

11 6

No pseudopotential on this center.

12 7

No pseudopotential on this center.

13 6

No pseudopotential on this center.

14 6

No pseudopotential on this center.

15 6

No pseudopotential on this center.

16 7

No pseudopotential on this center.

17 6

No pseudopotential on this center.

18 7

No pseudopotential on this center.

19 7

No pseudopotential on this center.

20 6

No pseudopotential on this center.

21 6

No pseudopotential on this center.

22 6

No pseudopotential on this center.

23 6

No pseudopotential on this center.

24 7

No pseudopotential on this center.

25 30 12

F and up

1 386.7379660 -18.00000000 0.00000000

2 72.8587359 -124.35274030 0.00000000

2 15.9066170 -30.66018220 0.00000000

2 4.3502340 -10.63589890 0.00000000

2 1.2842199 -0.76836230 0.00000000

S - F

0 19.0867858 3.00000000 0.00000000

1 5.0231080 22.52342250 0.00000000

2 1.2701744 48.44659420 0.00000000

2 1.0671287 -44.55601190 0.00000000

2 0.9264190 12.99839580 0.00000000

P - F

0 43.4927750 5.00000000 0.00000000

1 20.8692669 20.74355890 0.00000000

2 21.7118378 90.30271580 0.00000000

2 6.3616915 74.66103160 0.00000000

2 1.2291195 9.88944240 0.00000000

D - F

2 13.5851800 -4.84903590 0.00000000

2 9.8373050 3.69133790 0.00000000

2 0.8373113 -0.50373190 0.00000000

26 6

No pseudopotential on this center.

27 1

No pseudopotential on this center.

28 6

No pseudopotential on this center.

29 1

No pseudopotential on this center.

30 6

No pseudopotential on this center.

31 1

No pseudopotential on this center.

32 6

No pseudopotential on this center.

33 1

No pseudopotential on this center.

34 1

No pseudopotential on this center.

35 1

No pseudopotential on this center.

36 1

No pseudopotential on this center.

37 1

No pseudopotential on this center.

38 1

No pseudopotential on this center.

39 1

No pseudopotential on this center.

40 1

No pseudopotential on this center.

41 1

No pseudopotential on this center.

42 1

No pseudopotential on this center.

43 1

No pseudopotential on this center.

44 1

No pseudopotential on this center.

45 1

No pseudopotential on this center.

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

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

There are 229 symmetry adapted cartesian basis functions of AG symmetry.

There are 82 symmetry adapted cartesian basis functions of BG symmetry.

There are 78 symmetry adapted cartesian basis functions of AU symmetry.

There are 218 symmetry adapted cartesian basis functions of BU symmetry.

There are 212 symmetry adapted basis functions of AG symmetry.

There are 82 symmetry adapted basis functions of BG symmetry.

There are 78 symmetry adapted basis functions of AU symmetry.

There are 204 symmetry adapted basis functions of BU symmetry.

576 basis functions, 1015 primitive gaussians, 607 cartesian basis functions

103 alpha electrons 102 beta electrons

nuclear repulsion energy 2759.9985592461 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= 45 NActive= 45 NUniq= 11 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1140368129 Hartrees.

Nuclear repulsion after empirical dispersion term = 2759.8845224332 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= 45.

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 = 45

GePol: Total number of spheres = 45

GePol: Number of exposed spheres = 45 (100.00%)

GePol: Number of points = 3558

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.58D-09

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 180

GePol: Fraction of low-weight points (<1% of avg) = 5.06%

GePol: Cavity surface area = 383.317 Ang\*\*2

GePol: Cavity volume = 379.762 Ang\*\*3

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

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

PCM non-electrostatic energy = -0.0106881579 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2759.8738342752 Hartrees.

Leave Link 301 at Tue Sep 17 13:48:12 2019, MaxMem= 2415919104 cpu: 3.0

(Enter /home/blab/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

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15315 LenP2D= 41224.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.84D-04 NBF= 212 82 78 204

NBsUse= 576 1.00D-06 EigRej= -1.00D+00 NBFU= 212 82 78 204

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= 594 594 594 594 594 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Tue Sep 17 13:48:13 2019, MaxMem= 2415919104 cpu: 14.5

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 13:48:13 2019, MaxMem= 2415919104 cpu: 1.3

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

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -1276.40505126296

JPrj=0 DoOrth=F DoCkMO=F.

Initial guess orbital symmetries:

Alpha Orbitals:

Occupied (EU) (EU) (BG) (AG) (BG) (EU) (EU) (AG) (BG) (EU)

(EU) (AG) (EU) (EU) (AG) (BG) (EU) (EU) (AG) (BG)

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Beta Orbitals:

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

Leave Link 401 at Tue Sep 17 13:48:14 2019, MaxMem= 2415919104 cpu: 20.6

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1142439 IEndB= 1142439 NGot= 2415919104 MDV= 2415162362

LenX= 2415162362 LenY= 2414793306

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:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

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

IRaf= 670000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 37978092.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.99D-15 for 3557.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.63D-15 for 3551 2673.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.10D-15 for 3557.

Iteration 1 A^-1\*A deviation from orthogonality is 2.33D-12 for 2196 2167.

E= -1275.24217726047

DIIS: error= 9.03D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.24217726047 IErMin= 1 ErrMin= 9.03D-02

ErrMax= 9.03D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.20D+00 BMatP= 4.20D+00

IDIUse=3 WtCom= 9.70D-02 WtEn= 9.03D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.022 Goal= None Shift= 0.000

Gap= 0.123 Goal= None Shift= 0.000

GapD= 0.022 DampG=0.250 DampE=0.250 DampFc=0.1250 IDamp=-1.

Damping current iteration by 1.25D-01

RMSDP=3.04D-03 MaxDP=1.28D-01 OVMax= 1.86D-01

Cycle 2 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 3.78D-04 CP: 9.96D-01

E= -1275.40815795737 Delta-E= -0.165980696892 Rises=F Damp=T

DIIS: error= 6.41D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.40815795737 IErMin= 2 ErrMin= 6.41D-02

ErrMax= 6.41D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.35D+00 BMatP= 4.20D+00

IDIUse=3 WtCom= 3.59D-01 WtEn= 6.41D-01

Coeff-Com: -0.279D+01 0.379D+01

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

Coeff: -0.100D+01 0.200D+01

Gap= 0.028 Goal= None Shift= 0.000

Gap= 0.116 Goal= None Shift= 0.000

RMSDP=1.80D-03 MaxDP=8.04D-02 DE=-1.66D-01 OVMax= 6.27D-02

Cycle 3 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 1.07D-03 CP: 9.78D-01 3.00D+00

E= -1275.83592377165 Delta-E= -0.427765814282 Rises=F Damp=F

DIIS: error= 4.59D-02 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1275.83592377165 IErMin= 3 ErrMin= 4.59D-02

ErrMax= 4.59D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.13D-01 BMatP= 2.35D+00

IDIUse=3 WtCom= 5.41D-01 WtEn= 4.59D-01

EnCoef did 100 forward-backward iterations

Coeff-Com: 0.209D+01-0.216D+01 0.107D+01

Coeff-En: 0.133D+00 0.354D-02 0.863D+00

Coeff: 0.119D+01-0.117D+01 0.975D+00

Gap= 0.033 Goal= None Shift= 0.000

Gap= 0.087 Goal= None Shift= 0.000

RMSDP=9.23D-04 MaxDP=4.35D-02 DE=-4.28D-01 OVMax= 5.72D-02

Cycle 4 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 4.28D-04 CP: 9.86D-01 3.00D+00 2.35D-01

E= -1275.99007909583 Delta-E= -0.154155324179 Rises=F Damp=F

DIIS: error= 1.34D-02 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.99007909583 IErMin= 4 ErrMin= 1.34D-02

ErrMax= 1.34D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.13D-01 BMatP= 9.13D-01

IDIUse=3 WtCom= 8.66D-01 WtEn= 1.34D-01

Coeff-Com: -0.918D-01 0.148D+00 0.267D+00 0.677D+00

Coeff-En: 0.000D+00 0.000D+00 0.439D-01 0.956D+00

Coeff: -0.795D-01 0.128D+00 0.237D+00 0.714D+00

Gap= 0.033 Goal= None Shift= 0.000

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=2.45D-04 MaxDP=1.41D-02 DE=-1.54D-01 OVMax= 2.93D-02

Cycle 5 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 9.34D-05 CP: 9.84D-01 3.00D+00 4.20D-01 7.45D-01

E= -1276.01099041545 Delta-E= -0.020911319619 Rises=F Damp=F

DIIS: error= 1.98D-03 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1276.01099041545 IErMin= 5 ErrMin= 1.98D-03

ErrMax= 1.98D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.52D-03 BMatP= 1.13D-01

IDIUse=3 WtCom= 9.80D-01 WtEn= 1.98D-02

Coeff-Com: -0.170D+00 0.199D+00 0.783D-01 0.430D+00 0.462D+00

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

Coeff: -0.166D+00 0.195D+00 0.768D-01 0.421D+00 0.473D+00

Gap= 0.033 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=5.59D-05 MaxDP=2.78D-03 DE=-2.09D-02 OVMax= 9.68D-03

Cycle 6 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 2.62D-05 CP: 9.84D-01 3.00D+00 4.03D-01 7.85D-01 5.46D-01

E= -1276.01245137134 Delta-E= -0.001460955891 Rises=F Damp=F

DIIS: error= 4.70D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1276.01245137134 IErMin= 6 ErrMin= 4.70D-04

ErrMax= 4.70D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.84D-04 BMatP= 6.52D-03

IDIUse=3 WtCom= 9.95D-01 WtEn= 4.70D-03

Coeff-Com: -0.925D-01 0.106D+00 0.234D-01 0.181D+00 0.231D+00 0.551D+00

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

Coeff: -0.920D-01 0.106D+00 0.233D-01 0.180D+00 0.230D+00 0.553D+00

Gap= 0.034 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=1.34D-05 MaxDP=7.52D-04 DE=-1.46D-03 OVMax= 2.99D-03

Cycle 7 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 1.15D-05 CP: 9.84D-01 3.00D+00 4.06D-01 7.86D-01 5.85D-01

CP: 8.27D-01

E= -1276.01249394535 Delta-E= -0.000042574014 Rises=F Damp=F

DIIS: error= 2.66D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1276.01249394535 IErMin= 7 ErrMin= 2.66D-04

ErrMax= 2.66D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.57D-05 BMatP= 1.84D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 2.66D-03

Coeff-Com: -0.269D-01 0.301D-01-0.419D-02 0.180D-01 0.281D-01 0.316D+00

Coeff-Com: 0.639D+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: -0.268D-01 0.300D-01-0.418D-02 0.180D-01 0.281D-01 0.315D+00

Coeff: 0.640D+00

Gap= 0.034 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=8.41D-06 MaxDP=5.02D-04 DE=-4.26D-05 OVMax= 3.73D-03

Cycle 8 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 6.43D-06 CP: 9.84D-01 3.00D+00 4.06D-01 7.89D-01 5.93D-01

CP: 1.02D+00 1.07D+00

E= -1276.01251345517 Delta-E= -0.000019509823 Rises=F Damp=F

DIIS: error= 1.50D-04 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1276.01251345517 IErMin= 8 ErrMin= 1.50D-04

ErrMax= 1.50D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.25D-06 BMatP= 4.57D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.50D-03

Coeff-Com: 0.368D-01-0.427D-01-0.660D-02-0.606D-01-0.810D-01-0.130D+00

Coeff-Com: 0.120D+00 0.116D+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: 0.367D-01-0.426D-01-0.659D-02-0.605D-01-0.808D-01-0.130D+00

Coeff: 0.119D+00 0.116D+01

Gap= 0.035 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=1.09D-05 MaxDP=4.53D-04 DE=-1.95D-05 OVMax= 6.91D-03

Cycle 9 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 5.15D-06 CP: 9.84D-01 3.00D+00 4.06D-01 7.91D-01 6.04D-01

CP: 1.18D+00 1.68D+00 1.77D+00

E= -1276.01252439944 Delta-E= -0.000010944267 Rises=F Damp=F

DIIS: error= 1.10D-04 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1276.01252439944 IErMin= 9 ErrMin= 1.10D-04

ErrMax= 1.10D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.86D-06 BMatP= 7.25D-06

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.10D-03

Coeff-Com: 0.276D-01-0.318D-01-0.319D-02-0.396D-01-0.502D-01-0.129D+00

Coeff-Com: -0.601D-01 0.715D+00 0.571D+00

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

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

Coeff: 0.275D-01-0.318D-01-0.319D-02-0.396D-01-0.502D-01-0.129D+00

Coeff: -0.600D-01 0.714D+00 0.572D+00

Gap= 0.035 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=5.86D-06 MaxDP=2.29D-04 DE=-1.09D-05 OVMax= 4.24D-03

Cycle 10 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 2.77D-06 CP: 9.84D-01 3.00D+00 4.06D-01 7.92D-01 6.06D-01

CP: 1.25D+00 1.87D+00 2.33D+00 1.44D+00

E= -1276.01252788551 Delta-E= -0.000003486065 Rises=F Damp=F

DIIS: error= 7.38D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1276.01252788551 IErMin=10 ErrMin= 7.38D-05

ErrMax= 7.38D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.16D-06 BMatP= 3.86D-06

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

Coeff-Com: 0.421D-02-0.474D-02-0.282D-03-0.504D-02-0.164D-02-0.286D-01

Coeff-Com: -0.828D-01 0.690D-01 0.324D+00 0.726D+00

Coeff: 0.421D-02-0.474D-02-0.282D-03-0.504D-02-0.164D-02-0.286D-01

Coeff: -0.828D-01 0.690D-01 0.324D+00 0.726D+00

Gap= 0.035 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=6.27D-06 MaxDP=2.22D-04 DE=-3.49D-06 OVMax= 4.90D-03

Cycle 11 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 1.68D-06 CP: 9.84D-01 3.00D+00 4.06D-01 7.91D-01 6.09D-01

CP: 1.30D+00 2.09D+00 2.85D+00 2.20D+00 1.52D+00

E= -1276.01253058458 Delta-E= -0.000002699071 Rises=F Damp=F

DIIS: error= 7.48D-05 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1276.01253058458 IErMin=10 ErrMin= 7.38D-05

ErrMax= 7.48D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.94D-07 BMatP= 1.16D-06

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

Coeff-Com: -0.412D-02 0.481D-02 0.510D-03 0.619D-02 0.113D-01 0.155D-01

Coeff-Com: -0.372D-01-0.141D+00 0.467D-01 0.362D+00 0.735D+00

Coeff: -0.412D-02 0.481D-02 0.510D-03 0.619D-02 0.113D-01 0.155D-01

Coeff: -0.372D-01-0.141D+00 0.467D-01 0.362D+00 0.735D+00

Gap= 0.035 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=6.39D-06 MaxDP=2.45D-04 DE=-2.70D-06 OVMax= 5.10D-03

Cycle 12 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 2.67D-06 CP: 9.84D-01 3.00D+00 4.06D-01 7.91D-01 6.09D-01

CP: 1.34D+00 2.28D+00 3.00D+00 2.94D+00 2.34D+00

CP: 1.86D+00

E= -1276.01253301435 Delta-E= -0.000002429778 Rises=F Damp=F

DIIS: error= 7.16D-05 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1276.01253301435 IErMin=12 ErrMin= 7.16D-05

ErrMax= 7.16D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.23D-07 BMatP= 4.94D-07

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

Coeff-Com: -0.878D-03 0.979D-03 0.336D-03 0.198D-02 0.152D-02 0.945D-02

Coeff-Com: 0.150D-01-0.462D-01-0.730D-01-0.257D+00 0.363D+00 0.985D+00

Coeff: -0.878D-03 0.979D-03 0.336D-03 0.198D-02 0.152D-02 0.945D-02

Coeff: 0.150D-01-0.462D-01-0.730D-01-0.257D+00 0.363D+00 0.985D+00

Gap= 0.035 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=8.55D-06 MaxDP=3.26D-04 DE=-2.43D-06 OVMax= 6.84D-03

Cycle 13 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 5.13D-06 CP: 9.84D-01 3.00D+00 4.06D-01 7.91D-01 6.09D-01

CP: 1.40D+00 2.53D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.69D+00

E= -1276.01253608332 Delta-E= -0.000003068969 Rises=F Damp=F

DIIS: error= 6.96D-05 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1276.01253608332 IErMin=13 ErrMin= 6.96D-05

ErrMax= 6.96D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.21D-07 BMatP= 4.23D-07

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

Coeff-Com: 0.118D-02-0.144D-02 0.192D-03-0.347D-03-0.216D-02 0.552D-02

Coeff-Com: 0.291D-01 0.189D-01-0.780D-01-0.432D+00-0.573D-01-0.322D+00

Coeff-Com: 0.184D+01

Coeff: 0.118D-02-0.144D-02 0.192D-03-0.347D-03-0.216D-02 0.552D-02

Coeff: 0.291D-01 0.189D-01-0.780D-01-0.432D+00-0.573D-01-0.322D+00

Coeff: 0.184D+01

Gap= 0.035 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=1.83D-05 MaxDP=7.01D-04 DE=-3.07D-06 OVMax= 1.47D-02

Cycle 14 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 1.08D-05 CP: 9.84D-01 3.00D+00 4.06D-01 7.91D-01 6.08D-01

CP: 1.51D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00

E= -1276.01254202871 Delta-E= -0.000005945391 Rises=F Damp=F

DIIS: error= 5.92D-05 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1276.01254202871 IErMin=14 ErrMin= 5.92D-05

ErrMax= 5.92D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.36D-07 BMatP= 3.21D-07

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

Coeff-Com: 0.179D-02-0.209D-02 0.128D-04-0.125D-02-0.148D-03 0.257D-02

Coeff-Com: -0.231D-02 0.296D-01 0.242D-01-0.377D-01-0.135D+00-0.213D+01

Coeff-Com: 0.238D+01 0.872D+00

Coeff: 0.179D-02-0.209D-02 0.128D-04-0.125D-02-0.148D-03 0.257D-02

Coeff: -0.231D-02 0.296D-01 0.242D-01-0.377D-01-0.135D+00-0.213D+01

Coeff: 0.238D+01 0.872D+00

Gap= 0.035 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=2.16D-05 MaxDP=8.25D-04 DE=-5.95D-06 OVMax= 1.73D-02

Cycle 15 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 1.30D-05 CP: 9.84D-01 3.00D+00 4.05D-01 7.91D-01 6.08D-01

CP: 1.64D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.58D+00

E= -1276.01254818430 Delta-E= -0.000006155588 Rises=F Damp=F

DIIS: error= 5.18D-05 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1276.01254818430 IErMin=15 ErrMin= 5.18D-05

ErrMax= 5.18D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.39D-07 BMatP= 3.21D-07

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

Coeff-Com: -0.130D-02 0.158D-02-0.136D-03 0.943D-03 0.469D-02 0.605D-02

Coeff-Com: -0.401D-01 0.140D-02 0.782D-01 0.579D+00 0.110D+00-0.127D+01

Coeff-Com: -0.379D-01-0.126D+01 0.282D+01

Coeff: -0.130D-02 0.158D-02-0.136D-03 0.943D-03 0.469D-02 0.605D-02

Coeff: -0.401D-01 0.140D-02 0.782D-01 0.579D+00 0.110D+00-0.127D+01

Coeff: -0.379D-01-0.126D+01 0.282D+01

Gap= 0.035 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=4.82D-05 MaxDP=1.84D-03 DE=-6.16D-06 OVMax= 3.86D-02

Cycle 16 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 3.36D-05 CP: 9.84D-01 3.00D+00 4.05D-01 7.90D-01 6.06D-01

CP: 1.91D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

E= -1276.01255806144 Delta-E= -0.000009877137 Rises=F Damp=F

DIIS: error= 2.73D-05 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1276.01255806144 IErMin=16 ErrMin= 2.73D-05

ErrMax= 2.73D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.27D-07 BMatP= 2.39D-07

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

Coeff-Com: -0.208D-02 0.245D-02 0.106D-03 0.242D-02 0.465D-02 0.122D-01

Coeff-Com: -0.198D-01 0.671D-02-0.127D-01 0.497D+00 0.103D-01-0.215D+00

Coeff-Com: -0.607D+00-0.165D+01 0.219D+01 0.783D+00

Coeff: -0.208D-02 0.245D-02 0.106D-03 0.242D-02 0.465D-02 0.122D-01

Coeff: -0.198D-01 0.671D-02-0.127D-01 0.497D+00 0.103D-01-0.215D+00

Coeff: -0.607D+00-0.165D+01 0.219D+01 0.783D+00

Gap= 0.035 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=3.04D-05 MaxDP=1.15D-03 DE=-9.88D-06 OVMax= 2.43D-02

Cycle 17 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 1.60D-05 CP: 9.84D-01 3.00D+00 4.04D-01 7.89D-01 6.04D-01

CP: 2.07D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 1.76D+00

E= -1276.01256154259 Delta-E= -0.000003481150 Rises=F Damp=F

DIIS: error= 1.62D-05 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=17 EnMin= -1276.01256154259 IErMin=17 ErrMin= 1.62D-05

ErrMax= 1.62D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.88D-07 BMatP= 2.27D-07

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

Coeff-Com: 0.515D-03-0.637D-03 0.362D-03 0.738D-03-0.539D-03 0.112D-01

Coeff-Com: 0.228D-01 0.543D-01-0.121D+00 0.307D-01-0.275D+00 0.248D+00

Coeff-Com: 0.355D+00-0.314D+00-0.176D+00 0.284D+00 0.879D+00

Coeff: 0.515D-03-0.637D-03 0.362D-03 0.738D-03-0.539D-03 0.112D-01

Coeff: 0.228D-01 0.543D-01-0.121D+00 0.307D-01-0.275D+00 0.248D+00

Coeff: 0.355D+00-0.314D+00-0.176D+00 0.284D+00 0.879D+00

Gap= 0.035 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=1.08D-06 MaxDP=5.54D-05 DE=-3.48D-06 OVMax= 4.90D-04

Cycle 18 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 7.81D-07 CP: 9.84D-01 3.00D+00 4.04D-01 7.89D-01 6.02D-01

CP: 2.06D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 1.78D+00 1.01D+00

E= -1276.01256167336 Delta-E= -0.000000130773 Rises=F Damp=F

DIIS: error= 1.52D-05 at cycle 18 NSaved= 18.

NSaved=18 IEnMin=18 EnMin= -1276.01256167336 IErMin=18 ErrMin= 1.52D-05

ErrMax= 1.52D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.88D-08 BMatP= 1.88D-07

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

Coeff-Com: -0.145D-04-0.542D-06 0.177D-03 0.696D-03 0.526D-03 0.719D-02

Coeff-Com: 0.886D-02 0.280D-01-0.631D-01 0.849D-01-0.166D+00 0.181D-01

Coeff-Com: 0.132D+00-0.277D+00-0.821D-02 0.380D-01 0.592D+00 0.603D+00

Coeff: -0.145D-04-0.542D-06 0.177D-03 0.696D-03 0.526D-03 0.719D-02

Coeff: 0.886D-02 0.280D-01-0.631D-01 0.849D-01-0.166D+00 0.181D-01

Coeff: 0.132D+00-0.277D+00-0.821D-02 0.380D-01 0.592D+00 0.603D+00

Gap= 0.035 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=2.18D-05 MaxDP=8.22D-04 DE=-1.31D-07 OVMax= 1.75D-02

Cycle 19 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 9.37D-07 CP: 9.84D-01 3.00D+00 4.04D-01 7.88D-01 6.00D-01

CP: 2.18D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 2.32D+00 1.73D+00 8.77D-01

E= -1276.01256278293 Delta-E= -0.000001109564 Rises=F Damp=F

DIIS: error= 1.10D-05 at cycle 19 NSaved= 19.

NSaved=19 IEnMin=19 EnMin= -1276.01256278293 IErMin=19 ErrMin= 1.10D-05

ErrMax= 1.10D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.10D-07 BMatP= 6.88D-08

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

Coeff-Com: -0.171D-03 0.192D-03-0.395D-05 0.301D-03 0.717D-03 0.240D-02

Coeff-Com: 0.219D-02 0.247D-03-0.894D-02-0.134D-01-0.541D-01-0.235D+00

Coeff-Com: 0.268D+00 0.197D+00-0.142D+00-0.405D+00-0.138D+00 0.735D+00

Coeff-Com: 0.791D+00

Coeff: -0.171D-03 0.192D-03-0.395D-05 0.301D-03 0.717D-03 0.240D-02

Coeff: 0.219D-02 0.247D-03-0.894D-02-0.134D-01-0.541D-01-0.235D+00

Coeff: 0.268D+00 0.197D+00-0.142D+00-0.405D+00-0.138D+00 0.735D+00

Coeff: 0.791D+00

Gap= 0.035 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=7.20D-06 MaxDP=2.67D-04 DE=-1.11D-06 OVMax= 5.75D-03

Cycle 20 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 1.60D-07 CP: 9.84D-01 3.00D+00 4.03D-01 7.88D-01 5.99D-01

CP: 2.21D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 2.50D+00 1.96D+00 1.44D+00 1.47D+00

E= -1276.01256294970 Delta-E= -0.000000166777 Rises=F Damp=F

DIIS: error= 3.98D-06 at cycle 20 NSaved= 20.

NSaved=20 IEnMin=20 EnMin= -1276.01256294970 IErMin=20 ErrMin= 3.98D-06

ErrMax= 3.98D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.48D-08 BMatP= 6.88D-08

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

Coeff-Com: -0.141D-03 0.169D-03-0.690D-04-0.478D-04 0.314D-03 0.260D-04

Coeff-Com: -0.259D-02-0.269D-02 0.117D-01 0.805D-02-0.175D-02-0.204D+00

Coeff-Com: 0.129D+00 0.730D-01 0.857D-01-0.253D+00-0.245D+00 0.404D+00

Coeff-Com: 0.305D+00 0.693D+00

Coeff: -0.141D-03 0.169D-03-0.690D-04-0.478D-04 0.314D-03 0.260D-04

Coeff: -0.259D-02-0.269D-02 0.117D-01 0.805D-02-0.175D-02-0.204D+00

Coeff: 0.129D+00 0.730D-01 0.857D-01-0.253D+00-0.245D+00 0.404D+00

Coeff: 0.305D+00 0.693D+00

Gap= 0.035 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=6.63D-07 MaxDP=2.50D-05 DE=-1.67D-07 OVMax= 5.21D-04

Cycle 21 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

Restarting incremental Fock formation.

E= -1276.01256296176 Delta-E= -0.000000012054 Rises=F Damp=F

DIIS: error= 1.87D-06 at cycle 21 NSaved= 20.

NSaved=20 IEnMin=20 EnMin= -1276.01256296176 IErMin=20 ErrMin= 1.87D-06

ErrMax= 1.87D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.50D-09 BMatP= 1.48D-08

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

Coeff-Com: 0.391D-05-0.335D-04-0.151D-03-0.207D-03-0.616D-03-0.131D-02

Coeff-Com: 0.936D-03 0.653D-02 0.926D-02 0.296D-02-0.407D-01 0.236D-02

Coeff-Com: -0.405D-01 0.909D-01-0.209D-01-0.649D-01 0.239D-02-0.181D+00

Coeff-Com: 0.374D+00 0.860D+00

Coeff: 0.391D-05-0.335D-04-0.151D-03-0.207D-03-0.616D-03-0.131D-02

Coeff: 0.936D-03 0.653D-02 0.926D-02 0.296D-02-0.407D-01 0.236D-02

Coeff: -0.405D-01 0.909D-01-0.209D-01-0.649D-01 0.239D-02-0.181D+00

Coeff: 0.374D+00 0.860D+00

Gap= 0.035 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=2.85D-06 MaxDP=1.05D-04 DE=-1.21D-08 OVMax= 2.28D-03

Cycle 22 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 2.85D-06 CP: 1.00D+00

E= -1276.01256297583 Delta-E= -0.000000014079 Rises=F Damp=F

DIIS: error= 8.60D-07 at cycle 22 NSaved= 20.

NSaved=20 IEnMin=20 EnMin= -1276.01256297583 IErMin=20 ErrMin= 8.60D-07

ErrMax= 8.60D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.90D-10 BMatP= 2.50D-09

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

Coeff-Com: -0.330D-05-0.239D-04-0.639D-04-0.412D-04-0.304D-03 0.522D-03

Coeff-Com: 0.853D-03 0.692D-02 0.927D-03 0.236D-02-0.121D-01-0.339D-01

Coeff-Com: 0.422D-01 0.242D-01 0.692D-03-0.460D-01-0.165D+00 0.962D-01

Coeff-Com: 0.364D+00 0.718D+00

Coeff: -0.330D-05-0.239D-04-0.639D-04-0.412D-04-0.304D-03 0.522D-03

Coeff: 0.853D-03 0.692D-02 0.927D-03 0.236D-02-0.121D-01-0.339D-01

Coeff: 0.422D-01 0.242D-01 0.692D-03-0.460D-01-0.165D+00 0.962D-01

Coeff: 0.364D+00 0.718D+00

Gap= 0.035 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=9.03D-08 MaxDP=3.33D-06 DE=-1.41D-08 OVMax= 6.49D-05

Cycle 23 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 4.07D-08 CP: 1.00D+00 1.03D+00

E= -1276.01256297620 Delta-E= -0.000000000364 Rises=F Damp=F

DIIS: error= 2.96D-07 at cycle 23 NSaved= 20.

NSaved=20 IEnMin=20 EnMin= -1276.01256297620 IErMin=20 ErrMin= 2.96D-07

ErrMax= 2.96D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.58D-11 BMatP= 5.90D-10

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

Coeff-Com: 0.297D-05 0.250D-04 0.923D-04-0.193D-03-0.689D-04-0.551D-04

Coeff-Com: 0.596D-02 0.200D-02 0.596D-02-0.154D-01-0.195D-01 0.190D-01

Coeff-Com: 0.199D-01 0.124D-01-0.290D-01-0.574D-01-0.258D-01-0.123D-01

Coeff-Com: 0.461D+00 0.634D+00

Coeff: 0.297D-05 0.250D-04 0.923D-04-0.193D-03-0.689D-04-0.551D-04

Coeff: 0.596D-02 0.200D-02 0.596D-02-0.154D-01-0.195D-01 0.190D-01

Coeff: 0.199D-01 0.124D-01-0.290D-01-0.574D-01-0.258D-01-0.123D-01

Coeff: 0.461D+00 0.634D+00

Gap= 0.035 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=5.10D-07 MaxDP=1.89D-05 DE=-3.64D-10 OVMax= 4.08D-04

Cycle 24 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 6.18D-09 CP: 1.00D+00 1.21D+00 7.47D-01

E= -1276.01256297649 Delta-E= -0.000000000286 Rises=F Damp=F

DIIS: error= 1.15D-07 at cycle 24 NSaved= 20.

NSaved=20 IEnMin=20 EnMin= -1276.01256297649 IErMin=20 ErrMin= 1.15D-07

ErrMax= 1.15D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.04D-11 BMatP= 5.58D-11

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

Coeff-Com: -0.587D-05 0.319D-04 0.119D-03 0.208D-03-0.604D-03-0.726D-03

Coeff-Com: -0.263D-03 0.418D-02-0.163D-02-0.761D-05-0.299D-02 0.301D-02

Coeff-Com: 0.302D-02-0.997D-03-0.106D-02-0.145D-01-0.456D-01 0.147D-01

Coeff-Com: 0.151D+00 0.892D+00

Coeff: -0.587D-05 0.319D-04 0.119D-03 0.208D-03-0.604D-03-0.726D-03

Coeff: -0.263D-03 0.418D-02-0.163D-02-0.761D-05-0.299D-02 0.301D-02

Coeff: 0.302D-02-0.997D-03-0.106D-02-0.145D-01-0.456D-01 0.147D-01

Coeff: 0.151D+00 0.892D+00

Gap= 0.035 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=8.15D-09 MaxDP=5.59D-07 DE=-2.86D-10 OVMax= 3.24D-06

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

Error on total polarization charges = 0.06996

SCF Done: E(UB3LYP) = -1276.01256298 A.U. after 24 cycles

NFock= 24 Conv=0.82D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7695 S= 0.5097

<L.S>= 0.000000000000E+00

KE= 1.320937539836D+03 PE=-8.599277489597D+03 EE= 3.242453552509D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.71

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7695, after 0.7503

Leave Link 502 at Tue Sep 17 13:50:30 2019, MaxMem= 2415919104 cpu: 2407.4

(Enter /home/blab/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:

Occupied (EU) (EU) (EU) (EU) (EU) (EU) (EU) (EU) (EU) (EU)

(EU) (EU) (EU) (EU) (EU) (EU) (BU) (?A) (BU) (?A)

(BU) (?A) (BU) (?A) (BU) (?A) (BU) (?A) (?B) (?B)

(?B) (?B) (?B) (?B) (?B) (?B) (EU) (EU) (EU) (EU)

(?C) (?B) (?B) (?C) (?C) (?B) (?B) (?C) (BG) (?D)

(?D) (?D) (?E) (?E) (EG) (EG) (EU) (EU) (?E) (?E)

(?C) (?E) (?E) (?C) (?C) (?F) (EG) (EG) (?G) (?H)

(?H) (?F) (?G) (?F) (EG) (EG) (?G) (?G) (?H) (?H)

(?F) (?G) (?H) (?H) (?F) (?G) (?G) (?B) (?B) (?I)

(?I) (?G) (?B) (?B) (?F) (?G) (BG) (?I) (?F) (?I)

(?F) (?F) (?I)

Virtual (?I) (?F) (?F) (?F) (EU) (EU) (?I) (?I) (?J) (?F)

(?J) (?J) (EU) (EU) (EU) (EU) (EU) (EU) (?F) (?F)

(?I) (?I) (EU) (EG) (EU) (EU) (EU) (EG) (EG) (EG)

(?J) (?J) (EU) (EU) (?J) (?J) (AU) (?J) (?B) (?B)

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(EG) (EG) (?J) (?J) (EG) (?J) (EU) (EU) (?J) (?J)

(?J) (?J) (?J) (?J) (?J) (EG) (?J) (EG) (EG) (EG)

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Beta Orbitals:

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Unable to determine electronic state: an orbital has unidentified symmetry.

Alpha occ. eigenvalues -- -14.30197 -14.30197 -14.28553 -14.28552 -14.28384

Alpha occ. eigenvalues -- -14.28383 -14.28311 -14.28311 -10.22417 -10.22417

Alpha occ. eigenvalues -- -10.22113 -10.22113 -10.21589 -10.21589 -10.21550

Alpha occ. eigenvalues -- -10.21550 -10.17225 -10.17225 -10.16668 -10.16668

Alpha occ. eigenvalues -- -10.15775 -10.15775 -10.15626 -10.15626 -10.15578

Alpha occ. eigenvalues -- -10.15578 -10.15463 -10.15463 -0.98056 -0.96685

Alpha occ. eigenvalues -- -0.96591 -0.93933 -0.91657 -0.87608 -0.87481

Alpha occ. eigenvalues -- -0.84284 -0.78197 -0.77751 -0.77638 -0.77467

Alpha occ. eigenvalues -- -0.72928 -0.70126 -0.69993 -0.69010 -0.67685

Alpha occ. eigenvalues -- -0.66220 -0.66056 -0.60837 -0.58838 -0.57037

Alpha occ. eigenvalues -- -0.56022 -0.55700 -0.54998 -0.54967 -0.54066

Alpha occ. eigenvalues -- -0.54041 -0.52876 -0.52359 -0.51400 -0.51338

Alpha occ. eigenvalues -- -0.50000 -0.48847 -0.48785 -0.46944 -0.46702

Alpha occ. eigenvalues -- -0.44408 -0.43031 -0.42991 -0.42881 -0.42095

Alpha occ. eigenvalues -- -0.41993 -0.41723 -0.41510 -0.39879 -0.39495

Alpha occ. eigenvalues -- -0.39431 -0.38516 -0.38177 -0.37980 -0.37942

Alpha occ. eigenvalues -- -0.37455 -0.36248 -0.36034 -0.36014 -0.35910

Alpha occ. eigenvalues -- -0.35694 -0.35102 -0.30958 -0.30878 -0.30503

Alpha occ. eigenvalues -- -0.30170 -0.28860 -0.26209 -0.25785 -0.24871

Alpha occ. eigenvalues -- -0.24256 -0.23730 -0.23675 -0.23633 -0.23550

Alpha occ. eigenvalues -- -0.23335 -0.19430 -0.12594

Alpha virt. eigenvalues -- -0.09092 -0.03981 0.03980 0.04374 0.04949

Alpha virt. eigenvalues -- 0.04974 0.05853 0.05999 0.06140 0.07122

Alpha virt. eigenvalues -- 0.07288 0.07498 0.08554 0.08577 0.09736

Alpha virt. eigenvalues -- 0.10456 0.10474 0.10727 0.11042 0.11381

Alpha virt. eigenvalues -- 0.12467 0.12520 0.13337 0.14026 0.14056

Alpha virt. eigenvalues -- 0.14090 0.14124 0.14593 0.14628 0.14872

Alpha virt. eigenvalues -- 0.19775 0.21268 0.21695 0.21742 0.22463

Alpha virt. eigenvalues -- 0.22859 0.23167 0.23586 0.23696 0.23758

Alpha virt. eigenvalues -- 0.24337 0.24845 0.24917 0.27426 0.28665

Alpha virt. eigenvalues -- 0.28937 0.28984 0.30033 0.30508 0.31446

Alpha virt. eigenvalues -- 0.31510 0.31995 0.32096 0.32186 0.32235

Alpha virt. eigenvalues -- 0.32794 0.33246 0.33363 0.33430 0.33546

Alpha virt. eigenvalues -- 0.35736 0.36357 0.36423 0.37069 0.39008

Alpha virt. eigenvalues -- 0.39036 0.39245 0.40388 0.40403 0.40541

Alpha virt. eigenvalues -- 0.41671 0.41674 0.41731 0.42734 0.42994

Alpha virt. eigenvalues -- 0.44818 0.44898 0.45095 0.45266 0.45420

Alpha virt. eigenvalues -- 0.46716 0.47367 0.47472 0.48552 0.49531

Alpha virt. eigenvalues -- 0.50034 0.50736 0.50835 0.51025 0.51162

Alpha virt. eigenvalues -- 0.51187 0.52625 0.52832 0.52832 0.52926

Alpha virt. eigenvalues -- 0.54189 0.54601 0.54637 0.54998 0.55268

Alpha virt. eigenvalues -- 0.57700 0.57741 0.57814 0.57863 0.58390

Alpha virt. eigenvalues -- 0.58416 0.58704 0.59058 0.59120 0.59867

Alpha virt. eigenvalues -- 0.60079 0.60366 0.61253 0.61320 0.61381

Alpha virt. eigenvalues -- 0.63344 0.64089 0.64586 0.64625 0.64912

Alpha virt. eigenvalues -- 0.64933 0.64986 0.66503 0.66540 0.66737

Alpha virt. eigenvalues -- 0.69451 0.69521 0.69800 0.70140 0.70242

Alpha virt. eigenvalues -- 0.70737 0.70848 0.71693 0.72421 0.72951

Alpha virt. eigenvalues -- 0.74756 0.75083 0.75121 0.76431 0.76840

Alpha virt. eigenvalues -- 0.77409 0.77485 0.79388 0.79408 0.80382

Alpha virt. eigenvalues -- 0.81245 0.81410 0.82220 0.82298 0.82497

Alpha virt. eigenvalues -- 0.83006 0.83067 0.83673 0.84077 0.86556

Alpha virt. eigenvalues -- 0.86569 0.86639 0.88054 0.90067 0.90082

Alpha virt. eigenvalues -- 0.90362 0.91040 0.95911 0.98221 0.98257

Alpha virt. eigenvalues -- 0.98979 0.99398 1.01140 1.01207 1.02786

Alpha virt. eigenvalues -- 1.05078 1.05238 1.05342 1.06405 1.06420

Alpha virt. eigenvalues -- 1.08304 1.09248 1.10784 1.10859 1.11984

Alpha virt. eigenvalues -- 1.12476 1.15017 1.15275 1.15372 1.15398

Alpha virt. eigenvalues -- 1.16118 1.16203 1.16257 1.16577 1.17582

Alpha virt. eigenvalues -- 1.19737 1.20859 1.20915 1.21354 1.22323

Alpha virt. eigenvalues -- 1.23499 1.23594 1.25231 1.25851 1.29366

Alpha virt. eigenvalues -- 1.30803 1.30830 1.30887 1.32520 1.38884

Alpha virt. eigenvalues -- 1.38954 1.38959 1.40649 1.41194 1.42694

Alpha virt. eigenvalues -- 1.42738 1.42861 1.43850 1.44043 1.45534

Alpha virt. eigenvalues -- 1.47006 1.51061 1.51278 1.51390 1.51936

Alpha virt. eigenvalues -- 1.51984 1.52061 1.52165 1.53395 1.53411

Alpha virt. eigenvalues -- 1.53470 1.54395 1.55527 1.56195 1.56269

Alpha virt. eigenvalues -- 1.56882 1.57489 1.57611 1.58722 1.60047

Alpha virt. eigenvalues -- 1.61463 1.62436 1.62510 1.63857 1.64597

Alpha virt. eigenvalues -- 1.64631 1.64986 1.68502 1.69971 1.70019

Alpha virt. eigenvalues -- 1.70623 1.71117 1.71139 1.71452 1.72654

Alpha virt. eigenvalues -- 1.74204 1.74258 1.75803 1.77807 1.77829

Alpha virt. eigenvalues -- 1.78472 1.81481 1.81696 1.81750 1.82032

Alpha virt. eigenvalues -- 1.86655 1.88387 1.88476 1.89125 1.90365

Alpha virt. eigenvalues -- 1.92285 1.92322 1.92400 1.93669 1.96131

Alpha virt. eigenvalues -- 1.97177 1.98285 1.98464 1.98877 2.02406

Alpha virt. eigenvalues -- 2.02524 2.02624 2.02699 2.03879 2.04044

Alpha virt. eigenvalues -- 2.04395 2.04444 2.07337 2.08915 2.10467

Alpha virt. eigenvalues -- 2.11286 2.11319 2.15083 2.15107 2.16873

Alpha virt. eigenvalues -- 2.17516 2.17572 2.19392 2.19633 2.22623

Alpha virt. eigenvalues -- 2.28894 2.30660 2.30773 2.31046 2.31281

Alpha virt. eigenvalues -- 2.31397 2.34809 2.34905 2.35868 2.36110

Alpha virt. eigenvalues -- 2.36196 2.36920 2.39126 2.39829 2.39893

Alpha virt. eigenvalues -- 2.40684 2.40744 2.41079 2.41503 2.45388

Alpha virt. eigenvalues -- 2.48768 2.48795 2.48882 2.49487 2.49554

Alpha virt. eigenvalues -- 2.49768 2.50510 2.50730 2.56571 2.57512

Alpha virt. eigenvalues -- 2.57515 2.57569 2.59599 2.59627 2.61246

Alpha virt. eigenvalues -- 2.62280 2.62364 2.65171 2.65543 2.66731

Alpha virt. eigenvalues -- 2.68477 2.69128 2.72697 2.72746 2.73968

Alpha virt. eigenvalues -- 2.74597 2.74652 2.74923 2.78155 2.78231

Alpha virt. eigenvalues -- 2.79077 2.82108 2.85288 2.86159 2.86335

Alpha virt. eigenvalues -- 2.86381 2.86795 2.87100 2.87202 2.87411

Alpha virt. eigenvalues -- 2.93641 2.93701 2.95009 2.95776 2.97355

Alpha virt. eigenvalues -- 2.99180 2.99275 3.03764 3.05528 3.06239

Alpha virt. eigenvalues -- 3.06356 3.07439 3.13451 3.13740 3.13974

Alpha virt. eigenvalues -- 3.14108 3.14376 3.14583 3.15920 3.16054

Alpha virt. eigenvalues -- 3.17912 3.17966 3.18050 3.19000 3.22439

Alpha virt. eigenvalues -- 3.22535 3.23062 3.24108 3.26292 3.28089

Alpha virt. eigenvalues -- 3.30186 3.30268 3.30329 3.32289 3.32364

Alpha virt. eigenvalues -- 3.38224 3.39311 3.40410 3.40435 3.40887

Alpha virt. eigenvalues -- 3.55537 3.59781 3.59842 3.72236 3.74658

Alpha virt. eigenvalues -- 3.74749 3.74809 3.78470 3.80001 3.80404

Alpha virt. eigenvalues -- 3.80462 3.80938 3.82971 3.83750 3.83836

Alpha virt. eigenvalues -- 3.89076 3.89775 3.89829 3.89955 3.93063

Alpha virt. eigenvalues -- 4.06509 4.06784 4.07116 4.07362 4.13321

Alpha virt. eigenvalues -- 4.14350 4.14481 4.20860 4.30265 4.37353

Alpha virt. eigenvalues -- 4.37768 4.40064 4.48316 4.53603 4.63593

Alpha virt. eigenvalues -- 4.63605 5.01936 5.05095 5.05320 5.13772

Alpha virt. eigenvalues -- 5.17467 5.35269 5.35688 5.52671 7.80020

Alpha virt. eigenvalues -- 7.80038 7.91192 7.96887 8.24520 11.21145

Alpha virt. eigenvalues -- 23.45145 23.47409 23.47593 23.48809 23.67751

Alpha virt. eigenvalues -- 23.68311 23.68483 23.68555 23.84329 23.85187

Alpha virt. eigenvalues -- 23.85483 23.86480 23.89169 23.90088 23.90466

Alpha virt. eigenvalues -- 23.90478 24.11516 24.11894 24.12117 24.12711

Alpha virt. eigenvalues -- 35.58549 35.62890 35.63225 35.64154 35.69594

Alpha virt. eigenvalues -- 35.70350 35.71387 35.71558

Beta occ. eigenvalues -- -14.30318 -14.30318 -14.28354 -14.28353 -14.28246

Beta occ. eigenvalues -- -14.28246 -14.28150 -14.28150 -10.22465 -10.22465

Beta occ. eigenvalues -- -10.22139 -10.22139 -10.21373 -10.21373 -10.21357

Beta occ. eigenvalues -- -10.21356 -10.17265 -10.17265 -10.16512 -10.16512

Beta occ. eigenvalues -- -10.15773 -10.15773 -10.15637 -10.15637 -10.15624

Beta occ. eigenvalues -- -10.15624 -10.15352 -10.15352 -0.97830 -0.96513

Beta occ. eigenvalues -- -0.96307 -0.93746 -0.91347 -0.87599 -0.86923

Beta occ. eigenvalues -- -0.83988 -0.78084 -0.77680 -0.77467 -0.77338

Beta occ. eigenvalues -- -0.72685 -0.69989 -0.69829 -0.68931 -0.67590

Beta occ. eigenvalues -- -0.66015 -0.65909 -0.60663 -0.58599 -0.56981

Beta occ. eigenvalues -- -0.55962 -0.55660 -0.54890 -0.54825 -0.54029

Beta occ. eigenvalues -- -0.54012 -0.52793 -0.52307 -0.51244 -0.51176

Beta occ. eigenvalues -- -0.49911 -0.48790 -0.48656 -0.46872 -0.46575

Beta occ. eigenvalues -- -0.43881 -0.42835 -0.42675 -0.42453 -0.42054

Beta occ. eigenvalues -- -0.41950 -0.41497 -0.41472 -0.39725 -0.39279

Beta occ. eigenvalues -- -0.39105 -0.38445 -0.38135 -0.37953 -0.37853

Beta occ. eigenvalues -- -0.36947 -0.36177 -0.35986 -0.35922 -0.35641

Beta occ. eigenvalues -- -0.35127 -0.35023 -0.30893 -0.30774 -0.29947

Beta occ. eigenvalues -- -0.28992 -0.28693 -0.26268 -0.25367 -0.24421

Beta occ. eigenvalues -- -0.24046 -0.23640 -0.23278 -0.23162 -0.22972

Beta occ. eigenvalues -- -0.22615 -0.18104

Beta virt. eigenvalues -- -0.09211 -0.08019 -0.02633 0.04061 0.04976

Beta virt. eigenvalues -- 0.05012 0.05173 0.06162 0.06447 0.06609

Beta virt. eigenvalues -- 0.07298 0.07515 0.07620 0.08577 0.08590

Beta virt. eigenvalues -- 0.09756 0.10480 0.10485 0.10751 0.11651

Beta virt. eigenvalues -- 0.11939 0.12912 0.13101 0.13344 0.14071

Beta virt. eigenvalues -- 0.14097 0.14137 0.14158 0.14948 0.15027

Beta virt. eigenvalues -- 0.15062 0.19900 0.21350 0.21721 0.21873

Beta virt. eigenvalues -- 0.22602 0.22902 0.23408 0.23750 0.23804

Beta virt. eigenvalues -- 0.23902 0.24453 0.25013 0.25100 0.27516

Beta virt. eigenvalues -- 0.28774 0.28979 0.29107 0.30151 0.30656

Beta virt. eigenvalues -- 0.31582 0.31655 0.32052 0.32226 0.32275

Beta virt. eigenvalues -- 0.32343 0.32900 0.33393 0.33459 0.33543

Beta virt. eigenvalues -- 0.33639 0.35798 0.36470 0.36534 0.37182

Beta virt. eigenvalues -- 0.39123 0.39144 0.39371 0.40588 0.40637

Beta virt. eigenvalues -- 0.40883 0.41715 0.41813 0.41815 0.42847

Beta virt. eigenvalues -- 0.43255 0.44967 0.44981 0.45410 0.45412

Beta virt. eigenvalues -- 0.45665 0.46832 0.47627 0.47646 0.48639

Beta virt. eigenvalues -- 0.49631 0.50269 0.50867 0.50933 0.51117

Beta virt. eigenvalues -- 0.51260 0.51321 0.52860 0.52930 0.53069

Beta virt. eigenvalues -- 0.53237 0.54450 0.54634 0.54713 0.55044

Beta virt. eigenvalues -- 0.55360 0.57757 0.57794 0.57889 0.57946

Beta virt. eigenvalues -- 0.58451 0.58471 0.58887 0.59101 0.59183

Beta virt. eigenvalues -- 0.59907 0.60102 0.60491 0.61330 0.61399

Beta virt. eigenvalues -- 0.61494 0.63420 0.64166 0.64784 0.64865

Beta virt. eigenvalues -- 0.64994 0.65014 0.65112 0.66588 0.66593

Beta virt. eigenvalues -- 0.66820 0.69531 0.69846 0.69864 0.70176

Beta virt. eigenvalues -- 0.70380 0.70855 0.71242 0.71798 0.72526

Beta virt. eigenvalues -- 0.73278 0.74905 0.75180 0.75278 0.76512

Beta virt. eigenvalues -- 0.76950 0.77498 0.77568 0.79460 0.79530

Beta virt. eigenvalues -- 0.80460 0.81508 0.81540 0.82273 0.82899

Beta virt. eigenvalues -- 0.82980 0.83083 0.83169 0.83738 0.84168

Beta virt. eigenvalues -- 0.86626 0.86627 0.86732 0.88115 0.90128

Beta virt. eigenvalues -- 0.90147 0.90626 0.91135 0.96029 0.98282

Beta virt. eigenvalues -- 0.98301 0.99068 0.99476 1.01213 1.01332

Beta virt. eigenvalues -- 1.03033 1.05143 1.05410 1.05610 1.06476

Beta virt. eigenvalues -- 1.06558 1.08470 1.09312 1.11009 1.11205

Beta virt. eigenvalues -- 1.12058 1.12728 1.15092 1.15330 1.15426

Beta virt. eigenvalues -- 1.15520 1.16477 1.16498 1.16588 1.16854

Beta virt. eigenvalues -- 1.17896 1.19855 1.20914 1.20981 1.21748

Beta virt. eigenvalues -- 1.22439 1.23781 1.23912 1.25293 1.25906

Beta virt. eigenvalues -- 1.29444 1.30912 1.30994 1.31104 1.32637

Beta virt. eigenvalues -- 1.39135 1.39187 1.39284 1.40775 1.41559

Beta virt. eigenvalues -- 1.42768 1.42849 1.43144 1.43931 1.44374

Beta virt. eigenvalues -- 1.45650 1.47163 1.51136 1.51314 1.51479

Beta virt. eigenvalues -- 1.51964 1.52019 1.52102 1.52196 1.53450

Beta virt. eigenvalues -- 1.53501 1.53523 1.54485 1.55675 1.56311

Beta virt. eigenvalues -- 1.56363 1.57003 1.57660 1.57715 1.58907

Beta virt. eigenvalues -- 1.60220 1.61549 1.62581 1.62652 1.63916

Beta virt. eigenvalues -- 1.64715 1.64738 1.65113 1.68584 1.69988

Beta virt. eigenvalues -- 1.70152 1.70909 1.71175 1.71307 1.71535

Beta virt. eigenvalues -- 1.72731 1.74410 1.74630 1.75901 1.77890

Beta virt. eigenvalues -- 1.77987 1.78772 1.81621 1.81775 1.81935

Beta virt. eigenvalues -- 1.82132 1.86748 1.88490 1.88591 1.89429

Beta virt. eigenvalues -- 1.90494 1.92368 1.92562 1.92750 1.93958

Beta virt. eigenvalues -- 1.96296 1.97350 1.98540 1.98591 1.99078

Beta virt. eigenvalues -- 2.02583 2.02656 2.02975 2.03004 2.03953

Beta virt. eigenvalues -- 2.04333 2.04504 2.04818 2.07457 2.09073

Beta virt. eigenvalues -- 2.10800 2.11257 2.11602 2.15418 2.15458

Beta virt. eigenvalues -- 2.17113 2.17654 2.17903 2.19615 2.19690

Beta virt. eigenvalues -- 2.22984 2.28979 2.30696 2.30838 2.31325

Beta virt. eigenvalues -- 2.31354 2.31767 2.34886 2.35476 2.35896

Beta virt. eigenvalues -- 2.36120 2.36261 2.36949 2.39215 2.40047

Beta virt. eigenvalues -- 2.40277 2.40761 2.40833 2.41363 2.41734

Beta virt. eigenvalues -- 2.45487 2.48895 2.48913 2.49122 2.49512

Beta virt. eigenvalues -- 2.49803 2.49935 2.50763 2.50908 2.56695

Beta virt. eigenvalues -- 2.57550 2.57698 2.57930 2.59687 2.59835

Beta virt. eigenvalues -- 2.61540 2.62559 2.62689 2.65478 2.65714

Beta virt. eigenvalues -- 2.66942 2.68838 2.69214 2.73036 2.73152

Beta virt. eigenvalues -- 2.74347 2.74690 2.74934 2.75094 2.78273

Beta virt. eigenvalues -- 2.78892 2.79438 2.82534 2.85695 2.86475

Beta virt. eigenvalues -- 2.86546 2.86781 2.87150 2.87233 2.87285

Beta virt. eigenvalues -- 2.87487 2.93710 2.93773 2.95073 2.96117

Beta virt. eigenvalues -- 2.97411 2.99477 2.99708 3.04157 3.05609

Beta virt. eigenvalues -- 3.06285 3.06425 3.07492 3.13492 3.13782

Beta virt. eigenvalues -- 3.14004 3.14189 3.14438 3.14705 3.15960

Beta virt. eigenvalues -- 3.16161 3.17959 3.18038 3.18113 3.19026

Beta virt. eigenvalues -- 3.22477 3.22665 3.23120 3.24195 3.26347

Beta virt. eigenvalues -- 3.28138 3.30240 3.30336 3.30398 3.32353

Beta virt. eigenvalues -- 3.32440 3.38296 3.39360 3.40442 3.40511

Beta virt. eigenvalues -- 3.40946 3.55646 3.59876 3.59935 3.72335

Beta virt. eigenvalues -- 3.74744 3.74846 3.74913 3.78553 3.80096

Beta virt. eigenvalues -- 3.80496 3.80587 3.81042 3.83409 3.83688

Beta virt. eigenvalues -- 3.84654 3.89364 3.89740 3.90502 3.91145

Beta virt. eigenvalues -- 3.93460 4.06513 4.07002 4.07121 4.07571

Beta virt. eigenvalues -- 4.13429 4.14418 4.14640 4.20984 4.30384

Beta virt. eigenvalues -- 4.37477 4.37982 4.40246 4.48438 4.53682

Beta virt. eigenvalues -- 4.63660 4.63705 5.02098 5.05208 5.05537

Beta virt. eigenvalues -- 5.13916 5.17666 5.35404 5.35907 5.52849

Beta virt. eigenvalues -- 7.80044 7.80060 7.91192 7.96892 8.24526

Beta virt. eigenvalues -- 11.21159 23.45183 23.47438 23.47633 23.48842

Beta virt. eigenvalues -- 23.67770 23.68333 23.68503 23.68576 23.84405

Beta virt. eigenvalues -- 23.85203 23.85627 23.86543 23.89289 23.90125

Beta virt. eigenvalues -- 23.90600 23.90651 24.11567 24.11934 24.12183

Beta virt. eigenvalues -- 24.12767 35.58623 35.62896 35.63342 35.64205

Beta virt. eigenvalues -- 35.69603 35.70270 35.71653 35.71916

Condensed to atoms (all electrons):

1 2 3 4 5 6

1 C 4.707527 0.394435 -0.143255 -0.065736 0.439827 -0.001046

2 N 0.394435 7.117634 0.398709 -0.060402 -0.104844 -0.089287

3 C -0.143255 0.398709 4.676814 0.432424 -0.068334 0.556019

4 C -0.065736 -0.060402 0.432424 5.109610 0.601018 -0.083584

5 C 0.439827 -0.104844 -0.068334 0.601018 5.165534 0.005589

6 N -0.001046 -0.089287 0.556019 -0.083584 0.005589 6.655162

7 C -0.000903 -0.002705 -0.100593 0.003692 -0.000429 0.515261

8 N 0.000324 -0.020801 -0.003311 -0.000073 -0.000196 -0.081879

9 C -0.000002 0.000171 -0.000785 0.000014 -0.000003 0.001334

10 C -0.000003 -0.000070 0.000070 0.000018 0.000000 0.004096

11 C 0.000016 0.000291 0.004096 -0.000381 0.000010 -0.048820

12 N 0.516210 -0.076184 0.000310 0.003786 -0.043557 -0.000164

13 C 0.003129 -0.000082 0.000019 0.000020 -0.000432 -0.000000

14 C -0.000278 -0.000195 -0.000004 0.000000 0.000012 -0.000000

15 C -0.000743 0.000400 -0.000016 -0.000003 0.000021 -0.000001

16 N -0.001181 -0.022776 0.000226 -0.000078 0.000278 -0.000003

17 C -0.113044 -0.002424 -0.000567 0.000216 0.003285 -0.000033

18 N -0.000026 -0.000002 -0.000001 -0.000000 -0.000000 0.000000

19 N 0.000173 -0.003103 0.000205 0.000002 0.000003 -0.000002

20 C -0.000055 0.000205 -0.000010 -0.000000 -0.000000 -0.000001

21 C -0.000000 0.000002 -0.000000 0.000000 -0.000000 -0.000000

22 C -0.000000 0.000003 -0.000000 -0.000000 0.000000 -0.000000

23 C -0.000005 0.000173 -0.000055 -0.000000 -0.000000 -0.000026

24 N -0.000001 -0.000006 -0.000025 -0.000000 -0.000000 -0.000162

25 Zn -0.016386 0.126748 -0.018208 -0.000304 0.000102 -0.006149

26 C 0.010762 0.009642 -0.070453 0.256971 -0.061090 0.016523

27 H -0.051195 0.006690 0.010570 -0.046782 0.395452 -0.000012

28 C 0.000000 0.000001 0.000001 -0.000000 0.000000 -0.000023

29 H 0.000002 0.000087 0.000020 -0.000182 -0.000006 0.007509

30 C -0.000245 0.000063 0.000000 -0.000000 -0.000031 0.000000

31 H 0.000011 0.000001 0.000000 0.000000 -0.000000 -0.000000

32 C 0.000000 -0.000000 0.000000 -0.000000 -0.000000 -0.000000

33 H -0.000000 0.000000 -0.000000 -0.000000 -0.000000 0.000000

34 H 0.000195 -0.000243 0.006093 -0.043552 -0.005346 0.000097

35 H 0.000012 0.000429 -0.005399 -0.049136 -0.000298 0.005212

36 H 0.000012 0.000429 -0.005399 -0.049136 -0.000298 0.005212

37 H 0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000008

38 H 0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000008

39 H -0.000000 -0.000000 0.000001 0.000000 0.000000 -0.000011

40 H 0.000046 0.000014 -0.000000 -0.000000 -0.000014 0.000000

41 H 0.000046 0.000014 -0.000000 -0.000000 -0.000014 0.000000

42 H 0.000041 0.000000 0.000000 0.000000 -0.000001 0.000000

43 H -0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000000

44 H -0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000000

45 H 0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000000

7 8 9 10 11 12

1 C -0.000903 0.000324 -0.000002 -0.000003 0.000016 0.516210

2 N -0.002705 -0.020801 0.000171 -0.000070 0.000291 -0.076184

3 C -0.100593 -0.003311 -0.000785 0.000070 0.004096 0.000310

4 C 0.003692 -0.000073 0.000014 0.000018 -0.000381 0.003786

5 C -0.000429 -0.000196 -0.000003 0.000000 0.000010 -0.043557

6 N 0.515261 -0.081879 0.001334 0.004096 -0.048820 -0.000164

7 C 4.642894 0.421963 -0.140470 -0.057641 0.429877 -0.000017

8 N 0.421963 7.124086 0.367104 -0.067339 -0.096470 -0.000005

9 C -0.140470 0.367104 4.732494 0.436863 -0.077122 -0.000001

10 C -0.057641 -0.067339 0.436863 5.069397 0.604082 -0.000000

11 C 0.429877 -0.096470 -0.077122 0.604082 5.188213 -0.000000

12 N -0.000017 -0.000005 -0.000001 -0.000000 -0.000000 6.581114

13 C -0.000000 0.000002 -0.000000 0.000000 -0.000000 -0.075544

14 C -0.000000 0.000003 -0.000000 -0.000000 0.000000 0.004986

15 C -0.000003 0.000155 -0.000055 -0.000000 -0.000000 -0.001963

16 N 0.000155 -0.003117 0.000225 0.000002 0.000003 -0.084220

17 C -0.000055 0.000225 -0.000012 -0.000000 -0.000000 0.564904

18 N -0.000001 -0.000003 -0.000033 -0.000000 -0.000000 -0.000162

19 N 0.000400 -0.022776 -0.002424 -0.000082 -0.000195 -0.000006

20 C -0.000016 0.000226 -0.000567 0.000019 -0.000004 -0.000025

21 C -0.000003 -0.000078 0.000216 0.000020 0.000000 -0.000000

22 C 0.000021 0.000278 0.003285 -0.000432 0.000012 -0.000000

23 C -0.000743 -0.001181 -0.113044 0.003129 -0.000278 -0.000001

24 N -0.001963 -0.084220 0.564904 -0.075544 0.004986 0.000000

25 Zn -0.016750 0.127007 -0.018141 -0.000244 0.000240 -0.005758

26 C -0.000195 0.000067 0.000001 -0.000000 -0.000033 -0.000020

27 H 0.000010 0.000001 0.000000 0.000000 -0.000000 0.007072

28 C 0.010486 0.009418 -0.071214 0.257627 -0.058999 -0.000000

29 H -0.051783 0.006918 0.010566 -0.046440 0.395225 0.000000

30 C 0.000000 -0.000000 0.000000 -0.000000 -0.000000 0.015529

31 H 0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000010

32 C 0.000000 0.000001 0.000001 -0.000000 0.000000 0.000000

33 H 0.000002 0.000081 -0.000050 -0.000166 -0.000006 -0.000000

34 H 0.000042 0.000000 0.000000 0.000000 -0.000001 -0.000011

35 H 0.000024 0.000013 0.000000 0.000000 -0.000029 0.000009

36 H 0.000024 0.000013 0.000000 0.000000 -0.000029 0.000009

37 H -0.000098 0.000459 -0.005260 -0.046160 -0.000413 -0.000000

38 H -0.000098 0.000459 -0.005260 -0.046160 -0.000413 -0.000000

39 H 0.000194 -0.000251 0.006062 -0.043230 -0.005259 -0.000000

40 H 0.000000 0.000000 0.000000 -0.000000 0.000000 0.004284

41 H 0.000000 0.000000 0.000000 -0.000000 0.000000 0.004284

42 H 0.000000 -0.000000 0.000000 0.000000 0.000000 0.000074

43 H 0.000000 0.000000 -0.000001 0.000000 -0.000000 0.000000

44 H 0.000000 0.000000 -0.000001 0.000000 -0.000000 0.000000

45 H -0.000000 -0.000000 0.000001 0.000000 0.000000 0.000000

13 14 15 16 17 18

1 C 0.003129 -0.000278 -0.000743 -0.001181 -0.113044 -0.000026

2 N -0.000082 -0.000195 0.000400 -0.022776 -0.002424 -0.000002

3 C 0.000019 -0.000004 -0.000016 0.000226 -0.000567 -0.000001

4 C 0.000020 0.000000 -0.000003 -0.000078 0.000216 -0.000000

5 C -0.000432 0.000012 0.000021 0.000278 0.003285 -0.000000

6 N -0.000000 -0.000000 -0.000001 -0.000003 -0.000033 0.000000

7 C -0.000000 -0.000000 -0.000003 0.000155 -0.000055 -0.000001

8 N 0.000002 0.000003 0.000155 -0.003117 0.000225 -0.000003

9 C -0.000000 -0.000000 -0.000055 0.000225 -0.000012 -0.000033

10 C 0.000000 -0.000000 -0.000000 0.000002 -0.000000 -0.000000

11 C -0.000000 0.000000 -0.000000 0.000003 -0.000000 -0.000000

12 N -0.075544 0.004986 -0.001963 -0.084220 0.564904 -0.000162

13 C 5.069397 0.604082 -0.057641 -0.067339 0.436863 0.004096

14 C 0.604082 5.188213 0.429877 -0.096470 -0.077122 -0.048820

15 C -0.057641 0.429877 4.642894 0.421963 -0.140470 0.515261

16 N -0.067339 -0.096470 0.421963 7.124086 0.367104 -0.081879

17 C 0.436863 -0.077122 -0.140470 0.367104 4.732494 0.001334

18 N 0.004096 -0.048820 0.515261 -0.081879 0.001334 6.655162

19 N -0.000070 0.000291 -0.002705 -0.020801 0.000171 -0.089287

20 C 0.000070 0.004096 -0.100593 -0.003311 -0.000785 0.556019

21 C 0.000018 -0.000381 0.003692 -0.000073 0.000014 -0.083584

22 C 0.000000 0.000010 -0.000429 -0.000196 -0.000003 0.005589

23 C -0.000003 0.000016 -0.000903 0.000324 -0.000002 -0.001046

24 N -0.000000 -0.000000 -0.000017 -0.000005 -0.000001 -0.000164

25 Zn -0.000244 0.000240 -0.016750 0.127007 -0.018141 -0.006149

26 C -0.000000 0.000000 0.000000 0.000001 0.000001 -0.000000

27 H -0.000166 -0.000006 0.000002 0.000081 -0.000050 0.000000

28 C -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

29 H -0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000000

30 C 0.257627 -0.058999 0.010486 0.009418 -0.071214 -0.000023

31 H -0.046440 0.395225 -0.051783 0.006918 0.010566 0.007509

32 C -0.000000 -0.000033 -0.000195 0.000067 0.000001 0.016523

33 H 0.000000 -0.000000 0.000010 0.000001 0.000000 -0.000012

34 H 0.000000 0.000000 -0.000000 -0.000000 0.000001 -0.000000

35 H 0.000000 -0.000000 0.000000 0.000000 -0.000001 -0.000000

36 H 0.000000 -0.000000 0.000000 0.000000 -0.000001 -0.000000

37 H -0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

38 H -0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

39 H 0.000000 0.000000 0.000000 -0.000000 0.000000 0.000000

40 H -0.046160 -0.000413 -0.000098 0.000459 -0.005260 0.000008

41 H -0.046160 -0.000413 -0.000098 0.000459 -0.005260 0.000008

42 H -0.043230 -0.005259 0.000194 -0.000251 0.006062 -0.000011

43 H 0.000000 -0.000029 0.000024 0.000013 0.000000 0.005212

44 H 0.000000 -0.000029 0.000024 0.000013 0.000000 0.005212

45 H 0.000000 -0.000001 0.000042 0.000000 0.000000 0.000097

19 20 21 22 23 24

1 C 0.000173 -0.000055 -0.000000 -0.000000 -0.000005 -0.000001

2 N -0.003103 0.000205 0.000002 0.000003 0.000173 -0.000006

3 C 0.000205 -0.000010 -0.000000 -0.000000 -0.000055 -0.000025

4 C 0.000002 -0.000000 0.000000 -0.000000 -0.000000 -0.000000

5 C 0.000003 -0.000000 -0.000000 0.000000 -0.000000 -0.000000

6 N -0.000002 -0.000001 -0.000000 -0.000000 -0.000026 -0.000162

7 C 0.000400 -0.000016 -0.000003 0.000021 -0.000743 -0.001963

8 N -0.022776 0.000226 -0.000078 0.000278 -0.001181 -0.084220

9 C -0.002424 -0.000567 0.000216 0.003285 -0.113044 0.564904

10 C -0.000082 0.000019 0.000020 -0.000432 0.003129 -0.075544

11 C -0.000195 -0.000004 0.000000 0.000012 -0.000278 0.004986

12 N -0.000006 -0.000025 -0.000000 -0.000000 -0.000001 0.000000

13 C -0.000070 0.000070 0.000018 0.000000 -0.000003 -0.000000

14 C 0.000291 0.004096 -0.000381 0.000010 0.000016 -0.000000

15 C -0.002705 -0.100593 0.003692 -0.000429 -0.000903 -0.000017

16 N -0.020801 -0.003311 -0.000073 -0.000196 0.000324 -0.000005

17 C 0.000171 -0.000785 0.000014 -0.000003 -0.000002 -0.000001

18 N -0.089287 0.556019 -0.083584 0.005589 -0.001046 -0.000164

19 N 7.117634 0.398709 -0.060402 -0.104844 0.394435 -0.076184

20 C 0.398709 4.676814 0.432424 -0.068334 -0.143255 0.000310

21 C -0.060402 0.432424 5.109610 0.601018 -0.065736 0.003786

22 C -0.104844 -0.068334 0.601018 5.165534 0.439827 -0.043557

23 C 0.394435 -0.143255 -0.065736 0.439827 4.707527 0.516210

24 N -0.076184 0.000310 0.003786 -0.043557 0.516210 6.581114

25 Zn 0.126748 -0.018208 -0.000304 0.000102 -0.016386 -0.005758

26 C -0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000000

27 H 0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000

28 C 0.000063 0.000000 -0.000000 -0.000031 -0.000245 0.015529

29 H 0.000001 0.000000 0.000000 -0.000000 0.000011 -0.000010

30 C 0.000001 0.000001 -0.000000 0.000000 0.000000 -0.000000

31 H 0.000087 0.000020 -0.000182 -0.000006 0.000002 0.000000

32 C 0.009642 -0.070453 0.256971 -0.061090 0.010762 -0.000020

33 H 0.006690 0.010570 -0.046782 0.395452 -0.051195 0.007072

34 H -0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

35 H 0.000000 0.000000 0.000000 -0.000000 -0.000000 0.000000

36 H 0.000000 0.000000 0.000000 -0.000000 -0.000000 0.000000

37 H 0.000014 -0.000000 -0.000000 -0.000014 0.000046 0.004284

38 H 0.000014 -0.000000 -0.000000 -0.000014 0.000046 0.004284

39 H 0.000000 0.000000 0.000000 -0.000001 0.000041 0.000074

40 H 0.000000 -0.000000 0.000000 -0.000000 0.000000 -0.000000

41 H 0.000000 -0.000000 0.000000 -0.000000 0.000000 -0.000000

42 H -0.000000 0.000001 0.000000 0.000000 -0.000000 -0.000000

43 H 0.000429 -0.005399 -0.049136 -0.000298 0.000012 0.000009

44 H 0.000429 -0.005399 -0.049136 -0.000298 0.000012 0.000009

45 H -0.000243 0.006093 -0.043552 -0.005346 0.000195 -0.000011

25 26 27 28 29 30

1 C -0.016386 0.010762 -0.051195 0.000000 0.000002 -0.000245

2 N 0.126748 0.009642 0.006690 0.000001 0.000087 0.000063

3 C -0.018208 -0.070453 0.010570 0.000001 0.000020 0.000000

4 C -0.000304 0.256971 -0.046782 -0.000000 -0.000182 -0.000000

5 C 0.000102 -0.061090 0.395452 0.000000 -0.000006 -0.000031

6 N -0.006149 0.016523 -0.000012 -0.000023 0.007509 0.000000

7 C -0.016750 -0.000195 0.000010 0.010486 -0.051783 0.000000

8 N 0.127007 0.000067 0.000001 0.009418 0.006918 -0.000000

9 C -0.018141 0.000001 0.000000 -0.071214 0.010566 0.000000

10 C -0.000244 -0.000000 0.000000 0.257627 -0.046440 -0.000000

11 C 0.000240 -0.000033 -0.000000 -0.058999 0.395225 -0.000000

12 N -0.005758 -0.000020 0.007072 -0.000000 0.000000 0.015529

13 C -0.000244 -0.000000 -0.000166 -0.000000 -0.000000 0.257627

14 C 0.000240 0.000000 -0.000006 -0.000000 -0.000000 -0.058999

15 C -0.016750 0.000000 0.000002 0.000000 0.000000 0.010486

16 N 0.127007 0.000001 0.000081 -0.000000 0.000000 0.009418

17 C -0.018141 0.000001 -0.000050 0.000000 -0.000000 -0.071214

18 N -0.006149 -0.000000 0.000000 0.000000 -0.000000 -0.000023

19 N 0.126748 -0.000000 0.000000 0.000063 0.000001 0.000001

20 C -0.018208 0.000000 -0.000000 0.000000 0.000000 0.000001

21 C -0.000304 -0.000000 -0.000000 -0.000000 0.000000 -0.000000

22 C 0.000102 -0.000000 -0.000000 -0.000031 -0.000000 0.000000

23 C -0.016386 0.000000 -0.000000 -0.000245 0.000011 0.000000

24 N -0.005758 0.000000 -0.000000 0.015529 -0.000010 -0.000000

25 Zn 10.247330 0.000435 -0.000123 0.000312 -0.000040 0.000312

26 C 0.000435 5.377634 -0.005042 -0.000000 0.000087 -0.000000

27 H -0.000123 -0.005042 0.474762 -0.000000 -0.000000 0.000080

28 C 0.000312 -0.000000 -0.000000 5.378219 -0.004986 0.000000

29 H -0.000040 0.000087 -0.000000 -0.004986 0.475339 -0.000000

30 C 0.000312 -0.000000 0.000080 0.000000 -0.000000 5.378219

31 H -0.000040 -0.000000 -0.000000 -0.000000 0.000000 -0.004986

32 C 0.000435 0.000000 -0.000000 -0.000000 -0.000000 -0.000000

33 H -0.000123 -0.000000 0.000000 0.000080 -0.000000 -0.000000

34 H 0.000093 0.390131 0.001559 -0.000000 0.000001 -0.000000

35 H 0.000083 0.390223 -0.000159 -0.000000 0.000049 0.000000

36 H 0.000083 0.390223 -0.000159 -0.000000 0.000049 0.000000

37 H 0.000072 0.000000 0.000000 0.389551 -0.000147 0.000000

38 H 0.000072 0.000000 0.000000 0.389551 -0.000147 0.000000

39 H 0.000088 -0.000000 0.000000 0.389889 0.001565 -0.000000

40 H 0.000072 -0.000000 0.000045 0.000000 -0.000000 0.389551

41 H 0.000072 -0.000000 0.000045 0.000000 -0.000000 0.389551

42 H 0.000088 -0.000000 0.000000 -0.000000 -0.000000 0.389889

43 H 0.000083 0.000000 -0.000000 0.000000 0.000000 -0.000000

44 H 0.000083 0.000000 -0.000000 0.000000 0.000000 -0.000000

45 H 0.000093 0.000000 -0.000000 -0.000000 0.000000 -0.000000

31 32 33 34 35 36

1 C 0.000011 0.000000 -0.000000 0.000195 0.000012 0.000012

2 N 0.000001 -0.000000 0.000000 -0.000243 0.000429 0.000429

3 C 0.000000 0.000000 -0.000000 0.006093 -0.005399 -0.005399

4 C 0.000000 -0.000000 -0.000000 -0.043552 -0.049136 -0.049136

5 C -0.000000 -0.000000 -0.000000 -0.005346 -0.000298 -0.000298

6 N -0.000000 -0.000000 0.000000 0.000097 0.005212 0.005212

7 C 0.000000 0.000000 0.000002 0.000042 0.000024 0.000024

8 N 0.000000 0.000001 0.000081 0.000000 0.000013 0.000013

9 C -0.000000 0.000001 -0.000050 0.000000 0.000000 0.000000

10 C -0.000000 -0.000000 -0.000166 0.000000 0.000000 0.000000

11 C -0.000000 0.000000 -0.000006 -0.000001 -0.000029 -0.000029

12 N -0.000010 0.000000 -0.000000 -0.000011 0.000009 0.000009

13 C -0.046440 -0.000000 0.000000 0.000000 0.000000 0.000000

14 C 0.395225 -0.000033 -0.000000 0.000000 -0.000000 -0.000000

15 C -0.051783 -0.000195 0.000010 -0.000000 0.000000 0.000000

16 N 0.006918 0.000067 0.000001 -0.000000 0.000000 0.000000

17 C 0.010566 0.000001 0.000000 0.000001 -0.000001 -0.000001

18 N 0.007509 0.016523 -0.000012 -0.000000 -0.000000 -0.000000

19 N 0.000087 0.009642 0.006690 -0.000000 0.000000 0.000000

20 C 0.000020 -0.070453 0.010570 0.000000 0.000000 0.000000

21 C -0.000182 0.256971 -0.046782 0.000000 0.000000 0.000000

22 C -0.000006 -0.061090 0.395452 0.000000 -0.000000 -0.000000

23 C 0.000002 0.010762 -0.051195 0.000000 -0.000000 -0.000000

24 N 0.000000 -0.000020 0.007072 0.000000 0.000000 0.000000

25 Zn -0.000040 0.000435 -0.000123 0.000093 0.000083 0.000083

26 C -0.000000 0.000000 -0.000000 0.390131 0.390223 0.390223

27 H -0.000000 -0.000000 0.000000 0.001559 -0.000159 -0.000159

28 C -0.000000 -0.000000 0.000080 -0.000000 -0.000000 -0.000000

29 H 0.000000 -0.000000 -0.000000 0.000001 0.000049 0.000049

30 C -0.004986 -0.000000 -0.000000 -0.000000 0.000000 0.000000

31 H 0.475339 0.000087 -0.000000 0.000000 0.000000 0.000000

32 C 0.000087 5.377634 -0.005042 0.000000 0.000000 0.000000

33 H -0.000000 -0.005042 0.474762 -0.000000 -0.000000 -0.000000

34 H 0.000000 0.000000 -0.000000 0.474187 -0.027039 -0.027039

35 H 0.000000 0.000000 -0.000000 -0.027039 0.494881 -0.033887

36 H 0.000000 0.000000 -0.000000 -0.027039 -0.033887 0.494881

37 H -0.000000 -0.000000 0.000045 0.000000 0.000000 -0.000000

38 H -0.000000 -0.000000 0.000045 0.000000 -0.000000 0.000000

39 H -0.000000 -0.000000 0.000000 -0.000000 -0.000000 -0.000000

40 H -0.000147 0.000000 0.000000 -0.000000 0.000000 -0.000000

41 H -0.000147 0.000000 0.000000 -0.000000 -0.000000 0.000000

42 H 0.001565 -0.000000 0.000000 -0.000000 0.000000 0.000000

43 H 0.000049 0.390223 -0.000159 0.000000 -0.000000 0.000000

44 H 0.000049 0.390223 -0.000159 0.000000 0.000000 -0.000000

45 H 0.000001 0.390131 0.001559 0.000000 0.000000 0.000000

37 38 39 40 41 42

1 C 0.000000 0.000000 -0.000000 0.000046 0.000046 0.000041

2 N 0.000000 0.000000 -0.000000 0.000014 0.000014 0.000000

3 C -0.000000 -0.000000 0.000001 -0.000000 -0.000000 0.000000

4 C 0.000000 0.000000 0.000000 -0.000000 -0.000000 0.000000

5 C -0.000000 -0.000000 0.000000 -0.000014 -0.000014 -0.000001

6 N 0.000008 0.000008 -0.000011 0.000000 0.000000 0.000000

7 C -0.000098 -0.000098 0.000194 0.000000 0.000000 0.000000

8 N 0.000459 0.000459 -0.000251 0.000000 0.000000 -0.000000

9 C -0.005260 -0.005260 0.006062 0.000000 0.000000 0.000000

10 C -0.046160 -0.046160 -0.043230 -0.000000 -0.000000 0.000000

11 C -0.000413 -0.000413 -0.005259 0.000000 0.000000 0.000000

12 N -0.000000 -0.000000 -0.000000 0.004284 0.004284 0.000074

13 C -0.000000 -0.000000 0.000000 -0.046160 -0.046160 -0.043230

14 C 0.000000 0.000000 0.000000 -0.000413 -0.000413 -0.005259

15 C 0.000000 0.000000 0.000000 -0.000098 -0.000098 0.000194

16 N 0.000000 0.000000 -0.000000 0.000459 0.000459 -0.000251

17 C 0.000000 0.000000 0.000000 -0.005260 -0.005260 0.006062

18 N 0.000000 0.000000 0.000000 0.000008 0.000008 -0.000011

19 N 0.000014 0.000014 0.000000 0.000000 0.000000 -0.000000

20 C -0.000000 -0.000000 0.000000 -0.000000 -0.000000 0.000001

21 C -0.000000 -0.000000 0.000000 0.000000 0.000000 0.000000

22 C -0.000014 -0.000014 -0.000001 -0.000000 -0.000000 0.000000

23 C 0.000046 0.000046 0.000041 0.000000 0.000000 -0.000000

24 N 0.004284 0.004284 0.000074 -0.000000 -0.000000 -0.000000

25 Zn 0.000072 0.000072 0.000088 0.000072 0.000072 0.000088

26 C 0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000000

27 H 0.000000 0.000000 0.000000 0.000045 0.000045 0.000000

28 C 0.389551 0.389551 0.389889 0.000000 0.000000 -0.000000

29 H -0.000147 -0.000147 0.001565 -0.000000 -0.000000 -0.000000

30 C 0.000000 0.000000 -0.000000 0.389551 0.389551 0.389889

31 H -0.000000 -0.000000 -0.000000 -0.000147 -0.000147 0.001565

32 C -0.000000 -0.000000 -0.000000 0.000000 0.000000 -0.000000

33 H 0.000045 0.000045 0.000000 0.000000 0.000000 0.000000

34 H 0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000000

35 H 0.000000 -0.000000 -0.000000 0.000000 -0.000000 0.000000

36 H -0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000000

37 H 0.485676 -0.030712 -0.026842 0.000000 -0.000000 0.000000

38 H -0.030712 0.485676 -0.026842 -0.000000 0.000000 0.000000

39 H -0.026842 -0.026842 0.471868 0.000000 0.000000 0.000000

40 H 0.000000 -0.000000 0.000000 0.485676 -0.030712 -0.026842

41 H -0.000000 0.000000 0.000000 -0.030712 0.485676 -0.026842

42 H 0.000000 0.000000 0.000000 -0.026842 -0.026842 0.471868

43 H 0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000000

44 H -0.000000 0.000000 0.000000 -0.000000 0.000000 -0.000000

45 H -0.000000 -0.000000 -0.000000 0.000000 0.000000 -0.000000

43 44 45

1 C -0.000000 -0.000000 0.000000

2 N 0.000000 0.000000 -0.000000

3 C 0.000000 0.000000 0.000000

4 C 0.000000 0.000000 0.000000

5 C -0.000000 -0.000000 0.000000

6 N -0.000000 -0.000000 -0.000000

7 C 0.000000 0.000000 -0.000000

8 N 0.000000 0.000000 -0.000000

9 C -0.000001 -0.000001 0.000001

10 C 0.000000 0.000000 0.000000

11 C -0.000000 -0.000000 0.000000

12 N 0.000000 0.000000 0.000000

13 C 0.000000 0.000000 0.000000

14 C -0.000029 -0.000029 -0.000001

15 C 0.000024 0.000024 0.000042

16 N 0.000013 0.000013 0.000000

17 C 0.000000 0.000000 0.000000

18 N 0.005212 0.005212 0.000097

19 N 0.000429 0.000429 -0.000243

20 C -0.005399 -0.005399 0.006093

21 C -0.049136 -0.049136 -0.043552

22 C -0.000298 -0.000298 -0.005346

23 C 0.000012 0.000012 0.000195

24 N 0.000009 0.000009 -0.000011

25 Zn 0.000083 0.000083 0.000093

26 C 0.000000 0.000000 0.000000

27 H -0.000000 -0.000000 -0.000000

28 C 0.000000 0.000000 -0.000000

29 H 0.000000 0.000000 0.000000

30 C -0.000000 -0.000000 -0.000000

31 H 0.000049 0.000049 0.000001

32 C 0.390223 0.390223 0.390131

33 H -0.000159 -0.000159 0.001559

34 H 0.000000 0.000000 0.000000

35 H -0.000000 0.000000 0.000000

36 H 0.000000 -0.000000 0.000000

37 H 0.000000 -0.000000 -0.000000

38 H -0.000000 0.000000 -0.000000

39 H 0.000000 0.000000 -0.000000

40 H 0.000000 -0.000000 0.000000

41 H -0.000000 0.000000 0.000000

42 H -0.000000 -0.000000 -0.000000

43 H 0.494881 -0.033887 -0.027039

44 H -0.033887 0.494881 -0.027039

45 H -0.027039 -0.027039 0.474187

Atomic-Atomic Spin Densities.

1 2 3 4 5 6

1 C 0.173456 -0.028047 -0.005568 -0.014486 0.022141 0.001143

2 N -0.028047 0.022213 0.017689 0.002448 -0.001430 -0.003188

3 C -0.005568 0.017689 -0.016035 0.015689 -0.002093 -0.024496

4 C -0.014486 0.002448 0.015689 0.136662 -0.016752 -0.007032

5 C 0.022141 -0.001430 -0.002093 -0.016752 -0.039082 0.000238

6 N 0.001143 -0.003188 -0.024496 -0.007032 0.000238 0.241586

7 C -0.000091 0.000612 0.001748 0.000259 -0.000008 -0.017089

8 N -0.000112 0.000684 0.000909 0.000042 -0.000003 -0.004078

9 C 0.000010 -0.000091 -0.000121 -0.000005 0.000000 0.001047

10 C 0.000000 -0.000002 -0.000018 -0.000001 0.000000 0.000248

11 C -0.000005 0.000027 0.000267 0.000050 -0.000000 -0.006381

12 N -0.000257 0.000722 0.000042 0.000024 0.000126 0.000001

13 C -0.000370 0.000021 0.000000 0.000000 0.000005 -0.000000

14 C 0.000090 -0.000009 -0.000000 -0.000000 0.000000 0.000000

15 C 0.000057 -0.000032 -0.000000 -0.000000 0.000000 0.000000

16 N 0.002083 -0.000653 -0.000054 -0.000010 0.000027 0.000003

17 C -0.012730 0.001767 0.000086 0.000094 -0.000436 -0.000006

18 N -0.000006 0.000003 0.000000 0.000000 -0.000000 -0.000000

19 N 0.000010 -0.000035 -0.000003 -0.000000 0.000000 0.000003

20 C 0.000004 -0.000003 -0.000001 -0.000000 0.000000 0.000000

21 C 0.000000 -0.000000 -0.000000 -0.000000 0.000000 0.000000

22 C -0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000000

23 C -0.000002 0.000010 0.000004 0.000000 -0.000000 -0.000006

24 N 0.000000 -0.000000 -0.000000 -0.000000 0.000000 0.000001

25 Zn -0.000207 -0.000641 0.000306 0.000003 -0.000066 0.000130

26 C -0.000153 -0.000071 0.000689 -0.003152 0.001191 0.000005

27 H -0.000064 0.000012 -0.000081 0.000094 0.000709 -0.000001

28 C -0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000002

29 H -0.000000 -0.000001 -0.000016 0.000001 0.000000 -0.000070

30 C 0.000017 0.000000 -0.000000 0.000000 0.000002 0.000000

31 H -0.000000 -0.000000 0.000000 -0.000000 -0.000000 0.000000

32 C -0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000000

33 H 0.000000 -0.000000 -0.000000 -0.000000 0.000000 0.000000

34 H -0.000003 -0.000002 -0.000000 -0.000192 0.000088 -0.000006

35 H 0.000094 -0.000046 -0.000495 -0.003649 0.000275 0.000619

36 H 0.000094 -0.000046 -0.000495 -0.003649 0.000275 0.000619

37 H -0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000000

38 H -0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000000

39 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000000

40 H 0.000011 -0.000000 -0.000000 -0.000000 0.000002 0.000000

41 H 0.000011 -0.000000 -0.000000 -0.000000 0.000002 0.000000

42 H -0.000000 0.000000 -0.000000 0.000000 0.000000 0.000000

43 H -0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000000

44 H -0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000000

45 H -0.000000 -0.000000 -0.000000 -0.000000 -0.000000 0.000000

7 8 9 10 11 12

1 C -0.000091 -0.000112 0.000010 0.000000 -0.000005 -0.000257

2 N 0.000612 0.000684 -0.000091 -0.000002 0.000027 0.000722

3 C 0.001748 0.000909 -0.000121 -0.000018 0.000267 0.000042

4 C 0.000259 0.000042 -0.000005 -0.000001 0.000050 0.000024

5 C -0.000008 -0.000003 0.000000 0.000000 -0.000000 0.000126

6 N -0.017089 -0.004078 0.001047 0.000248 -0.006381 0.000001

7 C -0.033305 0.015361 -0.003619 -0.000426 0.009375 -0.000000

8 N 0.015361 0.046277 -0.032114 -0.001768 0.003120 0.000000

9 C -0.003619 -0.032114 0.158133 0.018008 -0.010770 0.000000

10 C -0.000426 -0.001768 0.018008 -0.034584 -0.014436 0.000000

11 C 0.009375 0.003120 -0.010770 -0.014436 0.100686 -0.000000

12 N -0.000000 0.000000 0.000000 0.000000 -0.000000 -0.072433

13 C 0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000221

14 C -0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000129

15 C -0.000001 -0.000002 0.000003 0.000000 -0.000000 0.000022

16 N -0.000002 -0.000043 0.000011 0.000000 -0.000000 0.000385

17 C 0.000003 0.000011 -0.000002 -0.000000 0.000000 0.005985

18 N 0.000000 0.000003 -0.000006 -0.000000 0.000000 0.000001

19 N -0.000032 -0.000653 0.001767 0.000021 -0.000009 -0.000000

20 C -0.000000 -0.000054 0.000086 0.000000 -0.000000 -0.000000

21 C -0.000000 -0.000010 0.000094 0.000000 -0.000000 -0.000000

22 C 0.000000 0.000027 -0.000436 0.000005 0.000000 0.000000

23 C 0.000057 0.002083 -0.012730 -0.000370 0.000090 0.000000

24 N 0.000022 0.000385 0.005985 0.000221 -0.000129 -0.000000

25 Zn 0.000210 -0.000891 -0.000181 -0.000061 0.000022 0.000141

26 C -0.000011 -0.000001 -0.000000 -0.000000 -0.000003 -0.000000

27 H 0.000000 0.000000 0.000000 -0.000000 0.000000 0.000079

28 C -0.000081 0.000082 -0.001348 0.001018 0.000624 0.000000

29 H 0.000363 -0.000055 -0.000118 0.000157 -0.000405 -0.000000

30 C -0.000000 -0.000000 0.000000 0.000000 -0.000000 0.000213

31 H 0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.000003

32 C -0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000000

33 H -0.000000 0.000000 -0.000005 0.000000 0.000000 0.000000

34 H -0.000000 -0.000000 -0.000000 -0.000000 0.000000 -0.000000

35 H -0.000030 -0.000003 0.000000 0.000000 -0.000014 -0.000000

36 H -0.000030 -0.000003 0.000000 0.000000 -0.000014 -0.000000

37 H -0.000011 0.000011 -0.000216 0.000683 0.000107 -0.000000

38 H -0.000011 0.000011 -0.000216 0.000683 0.000107 -0.000000

39 H 0.000009 0.000000 0.000030 0.000015 -0.000087 -0.000000

40 H -0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000046

41 H -0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000046

42 H 0.000000 -0.000000 -0.000000 -0.000000 0.000000 -0.000002

43 H 0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.000000

44 H 0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.000000

45 H -0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000000

13 14 15 16 17 18

1 C -0.000370 0.000090 0.000057 0.002083 -0.012730 -0.000006

2 N 0.000021 -0.000009 -0.000032 -0.000653 0.001767 0.000003

3 C 0.000000 -0.000000 -0.000000 -0.000054 0.000086 0.000000

4 C 0.000000 -0.000000 -0.000000 -0.000010 0.000094 0.000000

5 C 0.000005 0.000000 0.000000 0.000027 -0.000436 -0.000000

6 N -0.000000 0.000000 0.000000 0.000003 -0.000006 -0.000000

7 C 0.000000 -0.000000 -0.000001 -0.000002 0.000003 0.000000

8 N 0.000000 -0.000000 -0.000002 -0.000043 0.000011 0.000003

9 C -0.000000 0.000000 0.000003 0.000011 -0.000002 -0.000006

10 C -0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000000

11 C 0.000000 -0.000000 -0.000000 -0.000000 0.000000 0.000000

12 N 0.000221 -0.000129 0.000022 0.000385 0.005985 0.000001

13 C -0.034584 -0.014436 -0.000426 -0.001768 0.018008 0.000248

14 C -0.014436 0.100686 0.009375 0.003120 -0.010770 -0.006381

15 C -0.000426 0.009375 -0.033305 0.015361 -0.003619 -0.017089

16 N -0.001768 0.003120 0.015361 0.046277 -0.032114 -0.004078

17 C 0.018008 -0.010770 -0.003619 -0.032114 0.158133 0.001047

18 N 0.000248 -0.006381 -0.017089 -0.004078 0.001047 0.241586

19 N -0.000002 0.000027 0.000612 0.000684 -0.000091 -0.003188

20 C -0.000018 0.000267 0.001748 0.000909 -0.000121 -0.024496

21 C -0.000001 0.000050 0.000259 0.000042 -0.000005 -0.007032

22 C 0.000000 -0.000000 -0.000008 -0.000003 0.000000 0.000238

23 C 0.000000 -0.000005 -0.000091 -0.000112 0.000010 0.001143

24 N 0.000000 -0.000000 -0.000000 0.000000 0.000000 0.000001

25 Zn -0.000061 0.000022 0.000210 -0.000891 -0.000181 0.000130

26 C -0.000000 -0.000000 -0.000000 0.000000 -0.000000 -0.000000

27 H 0.000000 0.000000 -0.000000 0.000000 -0.000005 0.000000

28 C 0.000000 -0.000000 -0.000000 -0.000000 0.000000 0.000000

29 H -0.000000 0.000000 0.000000 0.000000 -0.000000 0.000000

30 C 0.001018 0.000624 -0.000081 0.000082 -0.001348 -0.000002

31 H 0.000157 -0.000405 0.000363 -0.000055 -0.000118 -0.000070

32 C -0.000000 -0.000003 -0.000011 -0.000001 -0.000000 0.000005

33 H -0.000000 0.000000 0.000000 0.000000 0.000000 -0.000001

34 H -0.000000 -0.000000 -0.000000 0.000000 -0.000000 0.000000

35 H -0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000000

36 H -0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000000

37 H 0.000000 -0.000000 -0.000000 -0.000000 0.000000 0.000000

38 H 0.000000 -0.000000 -0.000000 -0.000000 0.000000 0.000000

39 H -0.000000 0.000000 0.000000 -0.000000 -0.000000 0.000000

40 H 0.000683 0.000107 -0.000011 0.000011 -0.000216 -0.000000

41 H 0.000683 0.000107 -0.000011 0.000011 -0.000216 -0.000000

42 H 0.000015 -0.000087 0.000009 0.000000 0.000030 -0.000000

43 H 0.000000 -0.000014 -0.000030 -0.000003 0.000000 0.000619

44 H 0.000000 -0.000014 -0.000030 -0.000003 0.000000 0.000619

45 H -0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000006

19 20 21 22 23 24

1 C 0.000010 0.000004 0.000000 -0.000000 -0.000002 0.000000

2 N -0.000035 -0.000003 -0.000000 0.000000 0.000010 -0.000000

3 C -0.000003 -0.000001 -0.000000 0.000000 0.000004 -0.000000

4 C -0.000000 -0.000000 -0.000000 0.000000 0.000000 -0.000000

5 C 0.000000 0.000000 0.000000 -0.000000 -0.000000 0.000000

6 N 0.000003 0.000000 0.000000 -0.000000 -0.000006 0.000001

7 C -0.000032 -0.000000 -0.000000 0.000000 0.000057 0.000022

8 N -0.000653 -0.000054 -0.000010 0.000027 0.002083 0.000385

9 C 0.001767 0.000086 0.000094 -0.000436 -0.012730 0.005985

10 C 0.000021 0.000000 0.000000 0.000005 -0.000370 0.000221

11 C -0.000009 -0.000000 -0.000000 0.000000 0.000090 -0.000129

12 N -0.000000 -0.000000 -0.000000 0.000000 0.000000 -0.000000

13 C -0.000002 -0.000018 -0.000001 0.000000 0.000000 0.000000

14 C 0.000027 0.000267 0.000050 -0.000000 -0.000005 -0.000000

15 C 0.000612 0.001748 0.000259 -0.000008 -0.000091 -0.000000

16 N 0.000684 0.000909 0.000042 -0.000003 -0.000112 0.000000

17 C -0.000091 -0.000121 -0.000005 0.000000 0.000010 0.000000

18 N -0.003188 -0.024496 -0.007032 0.000238 0.001143 0.000001

19 N 0.022213 0.017689 0.002448 -0.001430 -0.028047 0.000722

20 C 0.017689 -0.016035 0.015689 -0.002093 -0.005568 0.000042

21 C 0.002448 0.015689 0.136662 -0.016752 -0.014486 0.000024

22 C -0.001430 -0.002093 -0.016752 -0.039082 0.022141 0.000126

23 C -0.028047 -0.005568 -0.014486 0.022141 0.173456 -0.000257

24 N 0.000722 0.000042 0.000024 0.000126 -0.000257 -0.072433

25 Zn -0.000641 0.000306 0.000003 -0.000066 -0.000207 0.000141

26 C 0.000000 0.000000 0.000000 -0.000000 -0.000000 -0.000000

27 H -0.000000 -0.000000 -0.000000 0.000000 0.000000 0.000000

28 C 0.000000 -0.000000 0.000000 0.000002 0.000017 0.000213

29 H -0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000003

30 C 0.000000 0.000000 0.000000 -0.000000 -0.000000 0.000000

31 H -0.000001 -0.000016 0.000001 0.000000 -0.000000 -0.000000

32 C -0.000071 0.000689 -0.003152 0.001191 -0.000153 -0.000000

33 H 0.000012 -0.000081 0.000094 0.000709 -0.000064 0.000079

34 H -0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000

35 H 0.000000 0.000000 0.000000 -0.000000 -0.000000 -0.000000

36 H 0.000000 0.000000 0.000000 -0.000000 -0.000000 -0.000000

37 H -0.000000 -0.000000 -0.000000 0.000002 0.000011 -0.000046

38 H -0.000000 -0.000000 -0.000000 0.000002 0.000011 -0.000046

39 H 0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000002

40 H 0.000000 0.000000 0.000000 -0.000000 -0.000000 -0.000000

41 H 0.000000 0.000000 0.000000 -0.000000 -0.000000 -0.000000

42 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000000

43 H -0.000046 -0.000495 -0.003649 0.000275 0.000094 -0.000000

44 H -0.000046 -0.000495 -0.003649 0.000275 0.000094 -0.000000

45 H -0.000002 -0.000000 -0.000192 0.000088 -0.000003 -0.000000

25 26 27 28 29 30

1 C -0.000207 -0.000153 -0.000064 -0.000000 -0.000000 0.000017

2 N -0.000641 -0.000071 0.000012 0.000000 -0.000001 0.000000

3 C 0.000306 0.000689 -0.000081 0.000000 -0.000016 -0.000000

4 C 0.000003 -0.003152 0.000094 0.000000 0.000001 0.000000

5 C -0.000066 0.001191 0.000709 -0.000000 0.000000 0.000002

6 N 0.000130 0.000005 -0.000001 -0.000002 -0.000070 0.000000

7 C 0.000210 -0.000011 0.000000 -0.000081 0.000363 -0.000000

8 N -0.000891 -0.000001 0.000000 0.000082 -0.000055 -0.000000

9 C -0.000181 -0.000000 0.000000 -0.001348 -0.000118 0.000000

10 C -0.000061 -0.000000 -0.000000 0.001018 0.000157 0.000000

11 C 0.000022 -0.000003 0.000000 0.000624 -0.000405 -0.000000

12 N 0.000141 -0.000000 0.000079 0.000000 -0.000000 0.000213

13 C -0.000061 -0.000000 0.000000 0.000000 -0.000000 0.001018

14 C 0.000022 -0.000000 0.000000 -0.000000 0.000000 0.000624

15 C 0.000210 -0.000000 -0.000000 -0.000000 0.000000 -0.000081

16 N -0.000891 0.000000 0.000000 -0.000000 0.000000 0.000082

17 C -0.000181 -0.000000 -0.000005 0.000000 -0.000000 -0.001348

18 N 0.000130 -0.000000 0.000000 0.000000 0.000000 -0.000002

19 N -0.000641 0.000000 -0.000000 0.000000 -0.000000 0.000000

20 C 0.000306 0.000000 -0.000000 -0.000000 0.000000 0.000000

21 C 0.000003 0.000000 -0.000000 0.000000 -0.000000 0.000000

22 C -0.000066 -0.000000 0.000000 0.000002 -0.000000 -0.000000

23 C -0.000207 -0.000000 0.000000 0.000017 -0.000000 -0.000000

24 N 0.000141 -0.000000 0.000000 0.000213 -0.000003 0.000000

25 Zn -0.000765 -0.000005 -0.000007 -0.000011 0.000006 -0.000011

26 C -0.000005 -0.011956 0.000137 0.000000 -0.000002 0.000000

27 H -0.000007 0.000137 0.000284 -0.000000 0.000000 0.000000

28 C -0.000011 0.000000 -0.000000 0.002118 0.000113 -0.000000

29 H 0.000006 -0.000002 0.000000 0.000113 -0.004391 0.000000

30 C -0.000011 0.000000 0.000000 -0.000000 0.000000 0.002118

31 H 0.000006 -0.000000 0.000000 0.000000 0.000000 0.000113

32 C -0.000005 0.000000 -0.000000 0.000000 -0.000000 0.000000

33 H -0.000007 -0.000000 -0.000000 0.000000 0.000000 -0.000000

34 H -0.000001 0.000472 0.000003 0.000000 -0.000000 0.000000

35 H -0.000002 0.001549 0.000002 -0.000000 -0.000001 0.000000

36 H -0.000002 0.001549 0.000002 -0.000000 -0.000001 0.000000

37 H 0.000000 -0.000000 -0.000000 -0.000205 0.000003 -0.000000

38 H 0.000000 -0.000000 -0.000000 -0.000205 0.000003 -0.000000

39 H 0.000001 0.000000 -0.000000 -0.000007 -0.000044 -0.000000

40 H 0.000000 0.000000 0.000000 -0.000000 0.000000 -0.000205

41 H 0.000000 0.000000 0.000000 -0.000000 0.000000 -0.000205

42 H 0.000001 -0.000000 0.000000 -0.000000 0.000000 -0.000007

43 H -0.000002 -0.000000 -0.000000 0.000000 0.000000 -0.000000

44 H -0.000002 -0.000000 -0.000000 0.000000 0.000000 -0.000000

45 H -0.000001 -0.000000 0.000000 0.000000 -0.000000 0.000000

31 32 33 34 35 36

1 C -0.000000 -0.000000 0.000000 -0.000003 0.000094 0.000094

2 N -0.000000 0.000000 -0.000000 -0.000002 -0.000046 -0.000046

3 C 0.000000 0.000000 -0.000000 -0.000000 -0.000495 -0.000495

4 C -0.000000 0.000000 -0.000000 -0.000192 -0.003649 -0.003649

5 C -0.000000 -0.000000 0.000000 0.000088 0.000275 0.000275

6 N 0.000000 -0.000000 0.000000 -0.000006 0.000619 0.000619

7 C 0.000000 -0.000000 -0.000000 -0.000000 -0.000030 -0.000030

8 N 0.000000 0.000000 0.000000 -0.000000 -0.000003 -0.000003

9 C -0.000000 -0.000000 -0.000005 -0.000000 0.000000 0.000000

10 C -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

11 C 0.000000 -0.000000 0.000000 0.000000 -0.000014 -0.000014

12 N -0.000003 -0.000000 0.000000 -0.000000 -0.000000 -0.000000

13 C 0.000157 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000

14 C -0.000405 -0.000003 0.000000 -0.000000 0.000000 0.000000

15 C 0.000363 -0.000011 0.000000 -0.000000 0.000000 0.000000

16 N -0.000055 -0.000001 0.000000 0.000000 0.000000 0.000000

17 C -0.000118 -0.000000 0.000000 -0.000000 -0.000000 -0.000000

18 N -0.000070 0.000005 -0.000001 0.000000 -0.000000 -0.000000

19 N -0.000001 -0.000071 0.000012 -0.000000 0.000000 0.000000

20 C -0.000016 0.000689 -0.000081 -0.000000 0.000000 0.000000

21 C 0.000001 -0.003152 0.000094 -0.000000 0.000000 0.000000

22 C 0.000000 0.001191 0.000709 -0.000000 -0.000000 -0.000000

23 C -0.000000 -0.000153 -0.000064 -0.000000 -0.000000 -0.000000

24 N -0.000000 -0.000000 0.000079 -0.000000 -0.000000 -0.000000

25 Zn 0.000006 -0.000005 -0.000007 -0.000001 -0.000002 -0.000002

26 C -0.000000 0.000000 -0.000000 0.000472 0.001549 0.001549

27 H 0.000000 -0.000000 -0.000000 0.000003 0.000002 0.000002

28 C 0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000000

29 H 0.000000 -0.000000 0.000000 -0.000000 -0.000001 -0.000001

30 C 0.000113 0.000000 -0.000000 0.000000 0.000000 0.000000

31 H -0.004391 -0.000002 0.000000 -0.000000 0.000000 0.000000

32 C -0.000002 -0.011956 0.000137 -0.000000 -0.000000 -0.000000

33 H 0.000000 0.000137 0.000284 0.000000 -0.000000 -0.000000

34 H -0.000000 -0.000000 0.000000 -0.000018 -0.000095 -0.000095

35 H 0.000000 -0.000000 -0.000000 -0.000095 0.010320 -0.003525

36 H 0.000000 -0.000000 -0.000000 -0.000095 -0.003525 0.010320

37 H 0.000000 0.000000 0.000000 -0.000000 -0.000000 0.000000

38 H 0.000000 0.000000 0.000000 -0.000000 0.000000 -0.000000

39 H 0.000000 -0.000000 0.000000 0.000000 0.000000 0.000000

40 H 0.000003 -0.000000 -0.000000 0.000000 0.000000 -0.000000

41 H 0.000003 -0.000000 -0.000000 0.000000 -0.000000 0.000000

42 H -0.000044 0.000000 -0.000000 -0.000000 0.000000 0.000000

43 H -0.000001 0.001549 0.000002 -0.000000 -0.000000 0.000000

44 H -0.000001 0.001549 0.000002 -0.000000 0.000000 -0.000000

45 H -0.000000 0.000472 0.000003 -0.000000 -0.000000 -0.000000

37 38 39 40 41 42

1 C -0.000000 -0.000000 0.000000 0.000011 0.000011 -0.000000

2 N 0.000000 0.000000 0.000000 -0.000000 -0.000000 0.000000

3 C 0.000000 0.000000 0.000000 -0.000000 -0.000000 -0.000000

4 C 0.000000 0.000000 0.000000 -0.000000 -0.000000 0.000000

5 C -0.000000 -0.000000 0.000000 0.000002 0.000002 0.000000

6 N -0.000000 -0.000000 -0.000000 0.000000 0.000000 0.000000

7 C -0.000011 -0.000011 0.000009 -0.000000 -0.000000 0.000000

8 N 0.000011 0.000011 0.000000 -0.000000 -0.000000 -0.000000

9 C -0.000216 -0.000216 0.000030 0.000000 0.000000 -0.000000

10 C 0.000683 0.000683 0.000015 0.000000 0.000000 -0.000000

11 C 0.000107 0.000107 -0.000087 -0.000000 -0.000000 0.000000

12 N -0.000000 -0.000000 -0.000000 -0.000046 -0.000046 -0.000002

13 C 0.000000 0.000000 -0.000000 0.000683 0.000683 0.000015

14 C -0.000000 -0.000000 0.000000 0.000107 0.000107 -0.000087

15 C -0.000000 -0.000000 0.000000 -0.000011 -0.000011 0.000009

16 N -0.000000 -0.000000 -0.000000 0.000011 0.000011 0.000000

17 C 0.000000 0.000000 -0.000000 -0.000216 -0.000216 0.000030

18 N 0.000000 0.000000 0.000000 -0.000000 -0.000000 -0.000000

19 N -0.000000 -0.000000 0.000000 0.000000 0.000000 0.000000

20 C -0.000000 -0.000000 -0.000000 0.000000 0.000000 0.000000

21 C -0.000000 -0.000000 0.000000 0.000000 0.000000 0.000000

22 C 0.000002 0.000002 0.000000 -0.000000 -0.000000 0.000000

23 C 0.000011 0.000011 -0.000000 -0.000000 -0.000000 0.000000

24 N -0.000046 -0.000046 -0.000002 -0.000000 -0.000000 -0.000000

25 Zn 0.000000 0.000000 0.000001 0.000000 0.000000 0.000001

26 C -0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000000

27 H -0.000000 -0.000000 -0.000000 0.000000 0.000000 0.000000

28 C -0.000205 -0.000205 -0.000007 -0.000000 -0.000000 -0.000000

29 H 0.000003 0.000003 -0.000044 0.000000 0.000000 0.000000

30 C -0.000000 -0.000000 -0.000000 -0.000205 -0.000205 -0.000007

31 H 0.000000 0.000000 0.000000 0.000003 0.000003 -0.000044

32 C 0.000000 0.000000 -0.000000 -0.000000 -0.000000 0.000000

33 H 0.000000 0.000000 0.000000 -0.000000 -0.000000 -0.000000

34 H -0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000000

35 H -0.000000 0.000000 0.000000 0.000000 -0.000000 0.000000

36 H 0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

37 H -0.001865 0.000587 0.000055 -0.000000 0.000000 0.000000

38 H 0.000587 -0.001865 0.000055 0.000000 -0.000000 0.000000

39 H 0.000055 0.000055 -0.000315 0.000000 0.000000 0.000000

40 H -0.000000 0.000000 0.000000 -0.001865 0.000587 0.000055

41 H 0.000000 -0.000000 0.000000 0.000587 -0.001865 0.000055

42 H 0.000000 0.000000 0.000000 0.000055 0.000055 -0.000315

43 H 0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

44 H -0.000000 0.000000 0.000000 0.000000 -0.000000 0.000000

45 H 0.000000 0.000000 -0.000000 -0.000000 -0.000000 0.000000

43 44 45

1 C -0.000000 -0.000000 -0.000000

2 N 0.000000 0.000000 -0.000000

3 C 0.000000 0.000000 -0.000000

4 C 0.000000 0.000000 -0.000000

5 C -0.000000 -0.000000 -0.000000

6 N -0.000000 -0.000000 0.000000

7 C 0.000000 0.000000 -0.000000

8 N 0.000000 0.000000 0.000000

9 C -0.000000 -0.000000 -0.000000

10 C -0.000000 -0.000000 -0.000000

11 C 0.000000 0.000000 -0.000000

12 N -0.000000 -0.000000 -0.000000

13 C 0.000000 0.000000 -0.000000

14 C -0.000014 -0.000014 0.000000

15 C -0.000030 -0.000030 -0.000000

16 N -0.000003 -0.000003 -0.000000

17 C 0.000000 0.000000 -0.000000

18 N 0.000619 0.000619 -0.000006

19 N -0.000046 -0.000046 -0.000002

20 C -0.000495 -0.000495 -0.000000

21 C -0.003649 -0.003649 -0.000192

22 C 0.000275 0.000275 0.000088

23 C 0.000094 0.000094 -0.000003

24 N -0.000000 -0.000000 -0.000000

25 Zn -0.000002 -0.000002 -0.000001

26 C -0.000000 -0.000000 -0.000000

27 H -0.000000 -0.000000 0.000000

28 C 0.000000 0.000000 0.000000

29 H 0.000000 0.000000 -0.000000

30 C -0.000000 -0.000000 0.000000

31 H -0.000001 -0.000001 -0.000000

32 C 0.001549 0.001549 0.000472

33 H 0.000002 0.000002 0.000003

34 H -0.000000 -0.000000 -0.000000

35 H -0.000000 0.000000 -0.000000

36 H 0.000000 -0.000000 -0.000000

37 H 0.000000 -0.000000 0.000000

38 H -0.000000 0.000000 0.000000

39 H 0.000000 0.000000 -0.000000

40 H -0.000000 0.000000 -0.000000

41 H 0.000000 -0.000000 -0.000000

42 H 0.000000 0.000000 0.000000

43 H 0.010320 -0.003525 -0.000095

44 H -0.003525 0.010320 -0.000095

45 H -0.000095 -0.000095 -0.000018

Mulliken charges and spin densities:

1 2

1 C 0.321335 0.137120

2 N -0.673017 0.011910

3 C 0.330838 -0.012048

4 C -0.008420 0.106441

5 C -0.326238 -0.034789

6 N -0.460828 0.183289

7 C 0.349423 -0.026729

8 N -0.677104 0.029218

9 C 0.311204 0.123193

10 C 0.008191 -0.030603

11 C -0.338598 0.082222

12 N -0.414922 -0.064954

13 C 0.008191 -0.030603

14 C -0.338598 0.082222

15 C 0.349423 -0.026729

16 N -0.677104 0.029218

17 C 0.311204 0.123193

18 N -0.460828 0.183289

19 N -0.673017 0.011910

20 C 0.330838 -0.012048

21 C -0.008420 0.106441

22 C -0.326238 -0.034789

23 C 0.321335 0.137120

24 N -0.414922 -0.064954

25 Zn 1.406206 -0.003273

26 C -0.705869 -0.009761

27 H 0.207326 0.001167

28 C -0.705231 0.002330

29 H 0.206312 -0.004461

30 C -0.705231 0.002330

31 H 0.206312 -0.004461

32 C -0.705869 -0.009761

33 H 0.207326 0.001167

34 H 0.230833 0.000150

35 H 0.225012 0.004999

36 H 0.225012 0.004999

37 H 0.229492 -0.000884

38 H 0.229492 -0.000884

39 H 0.232654 -0.000289

40 H 0.229492 -0.000884

41 H 0.229492 -0.000884

42 H 0.232654 -0.000289

43 H 0.225012 0.004999

44 H 0.225012 0.004999

45 H 0.230833 0.000150

Sum of Mulliken charges = -1.00000 1.00000

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

1 2

1 C 0.321335 0.137120

2 N -0.673017 0.011910

3 C 0.330838 -0.012048

4 C -0.008420 0.106441

5 C -0.118912 -0.033623

6 N -0.460828 0.183289

7 C 0.349423 -0.026729

8 N -0.677104 0.029218

9 C 0.311204 0.123193

10 C 0.008191 -0.030603

11 C -0.132287 0.077762

12 N -0.414922 -0.064954

13 C 0.008191 -0.030603

14 C -0.132287 0.077762

15 C 0.349423 -0.026729

16 N -0.677104 0.029218

17 C 0.311204 0.123193

18 N -0.460828 0.183289

19 N -0.673017 0.011910

20 C 0.330838 -0.012048

21 C -0.008420 0.106441

22 C -0.118912 -0.033623

23 C 0.321335 0.137120

24 N -0.414922 -0.064954

25 Zn 1.406206 -0.003273

26 C -0.025012 0.000388

28 C -0.013593 0.000273

30 C -0.013593 0.000273

32 C -0.025012 0.000388

Electronic spatial extent (au): <R\*\*2>= 11303.1994

Charge= -1.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 0.0000 Y= -0.0000 Z= -0.0000 Tot= 0.0000

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

XX= -203.1353 YY= -196.7391 ZZ= -177.1126

XY= -0.8494 XZ= 0.0000 YZ= 0.0000

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

XX= -10.8063 YY= -4.4101 ZZ= 15.2164

XY= -0.8494 XZ= 0.0000 YZ= 0.0000

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

XXX= -0.0000 YYY= 0.0000 ZZZ= -0.0000 XYY= -0.0000

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

YYZ= -0.0000 XYZ= 0.0000

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

XXXX= -7899.6529 YYYY= -7710.0299 ZZZZ= -217.9747 XXXY= -226.4066

XXXZ= -0.0000 YYYX= 205.9789 YYYZ= 0.0000 ZZZX= -0.0000

ZZZY= 0.0000 XXYY= -2645.3391 XXZZ= -1405.0747 YYZZ= -1398.5686

XXYZ= -0.0000 YYXZ= -0.0000 ZZXY= -0.2493

N-N= 2.759873834275D+03 E-N=-8.599277493231D+03 KE= 1.320937539836D+03

Symmetry AG KE= 6.505133725813D+02

Symmetry BG KE= 6.682453988885D+01

Symmetry AU KE= 2.215234147033D+01

Symmetry BU KE= 5.814472858957D+02

Isotropic Fermi Contact Couplings

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

1 C(13) 0.01021 11.48341 4.09757 3.83045

2 N(14) -0.00115 -0.37123 -0.13247 -0.12383

3 C(13) -0.00897 -10.08640 -3.59908 -3.36446

4 C(13) 0.00646 7.26249 2.59144 2.42251

5 C(13) -0.00778 -8.74726 -3.12124 -2.91777

6 N(14) 0.02079 6.71685 2.39674 2.24050

7 C(13) -0.00951 -10.69475 -3.81615 -3.56738

8 N(14) 0.00127 0.41140 0.14680 0.13723

9 C(13) 0.00907 10.19386 3.63742 3.40030

10 C(13) -0.00643 -7.22608 -2.57844 -2.41036

11 C(13) 0.00459 5.16030 1.84132 1.72129

12 N(14) -0.01062 -3.43063 -1.22413 -1.14433

13 C(13) -0.00643 -7.22608 -2.57844 -2.41036

14 C(13) 0.00459 5.16030 1.84132 1.72129

15 C(13) -0.00951 -10.69475 -3.81615 -3.56738

16 N(14) 0.00127 0.41140 0.14680 0.13723

17 C(13) 0.00907 10.19386 3.63742 3.40030

18 N(14) 0.02079 6.71685 2.39674 2.24050

19 N(14) -0.00115 -0.37123 -0.13247 -0.12383

20 C(13) -0.00897 -10.08640 -3.59908 -3.36446

21 C(13) 0.00646 7.26249 2.59144 2.42251

22 C(13) -0.00778 -8.74726 -3.12124 -2.91777

23 C(13) 0.01021 11.48341 4.09757 3.83045

24 N(14) -0.01062 -3.43063 -1.22413 -1.14433

25 Zn(67) 0.00000 0.00000 0.00000 0.00000

26 C(13) -0.00369 -4.15310 -1.48193 -1.38533

27 H(1) 0.00023 1.04664 0.37347 0.34912

28 C(13) 0.00051 0.57561 0.20539 0.19200

29 H(1) -0.00123 -5.51937 -1.96945 -1.84106

30 C(13) 0.00051 0.57561 0.20539 0.19200

31 H(1) -0.00123 -5.51937 -1.96945 -1.84106

32 C(13) -0.00369 -4.15310 -1.48193 -1.38533

33 H(1) 0.00023 1.04664 0.37347 0.34912

34 H(1) 0.00007 0.29685 0.10592 0.09902

35 H(1) 0.00228 10.20812 3.64251 3.40506

36 H(1) 0.00228 10.20812 3.64251 3.40506

37 H(1) -0.00028 -1.26026 -0.44969 -0.42038

38 H(1) -0.00028 -1.26026 -0.44969 -0.42038

39 H(1) -0.00010 -0.45676 -0.16298 -0.15236

40 H(1) -0.00028 -1.26026 -0.44969 -0.42038

41 H(1) -0.00028 -1.26026 -0.44969 -0.42038

42 H(1) -0.00010 -0.45676 -0.16298 -0.15236

43 H(1) 0.00228 10.20812 3.64251 3.40506

44 H(1) 0.00228 10.20812 3.64251 3.40506

45 H(1) 0.00007 0.29685 0.10592 0.09902

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

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

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

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

1 Atom -0.085024 -0.088578 0.173602

2 Atom -0.021794 -0.021179 0.042974

3 Atom -0.003105 0.012314 -0.009209

4 Atom -0.061518 -0.064158 0.125676

5 Atom 0.012058 0.013615 -0.025673

6 Atom -0.228445 -0.228665 0.457110

7 Atom 0.017296 0.011080 -0.028376

8 Atom -0.038272 -0.042026 0.080297

9 Atom -0.079316 -0.076757 0.156073

10 Atom 0.011031 0.011681 -0.022712

11 Atom -0.045193 -0.043623 0.088816

12 Atom 0.062479 0.053712 -0.116191

13 Atom 0.011031 0.011681 -0.022712

14 Atom -0.045193 -0.043623 0.088816

15 Atom 0.017296 0.011080 -0.028376

16 Atom -0.038272 -0.042026 0.080297

17 Atom -0.079316 -0.076757 0.156073

18 Atom -0.228445 -0.228665 0.457110

19 Atom -0.021794 -0.021179 0.042974

20 Atom -0.003105 0.012314 -0.009209

21 Atom -0.061518 -0.064158 0.125676

22 Atom 0.012058 0.013615 -0.025673

23 Atom -0.085024 -0.088578 0.173602

24 Atom 0.062479 0.053712 -0.116191

25 Atom 0.003221 -0.005654 0.002433

26 Atom 0.002763 -0.001754 -0.001009

27 Atom 0.002016 -0.000127 -0.001889

28 Atom -0.001025 0.001585 -0.000561

29 Atom 0.002043 -0.000290 -0.001753

30 Atom -0.001025 0.001585 -0.000561

31 Atom 0.002043 -0.000290 -0.001753

32 Atom 0.002763 -0.001754 -0.001009

33 Atom 0.002016 -0.000127 -0.001889

34 Atom 0.002260 -0.000999 -0.001261

35 Atom 0.002522 -0.000938 -0.001584

36 Atom 0.002522 -0.000938 -0.001584

37 Atom -0.000617 0.001502 -0.000885

38 Atom -0.000617 0.001502 -0.000885

39 Atom -0.000429 0.001287 -0.000859

40 Atom -0.000617 0.001502 -0.000885

41 Atom -0.000617 0.001502 -0.000885

42 Atom -0.000429 0.001287 -0.000859

43 Atom 0.002522 -0.000938 -0.001584

44 Atom 0.002522 -0.000938 -0.001584

45 Atom 0.002260 -0.000999 -0.001261

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

XY XZ YZ

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

1 Atom -0.000999 0.000000 -0.000000

2 Atom 0.001730 0.000000 0.000000

3 Atom 0.001617 0.000000 -0.000000

4 Atom -0.001114 -0.000000 0.000000

5 Atom 0.000255 -0.000000 0.000000

6 Atom -0.000155 -0.000000 0.000000

7 Atom -0.007548 0.000000 -0.000000

8 Atom -0.000547 -0.000000 0.000000

9 Atom 0.001203 0.000000 -0.000000

10 Atom -0.000433 -0.000000 -0.000000

11 Atom 0.001256 -0.000000 0.000000

12 Atom 0.004405 0.000000 -0.000000

13 Atom -0.000433 -0.000000 0.000000

14 Atom 0.001256 0.000000 0.000000

15 Atom -0.007548 -0.000000 -0.000000

16 Atom -0.000547 0.000000 -0.000000

17 Atom 0.001203 0.000000 0.000000

18 Atom -0.000155 -0.000000 -0.000000

19 Atom 0.001730 -0.000000 -0.000000

20 Atom 0.001617 -0.000000 0.000000

21 Atom -0.001114 -0.000000 -0.000000

22 Atom 0.000255 0.000000 -0.000000

23 Atom -0.000999 0.000000 -0.000000

24 Atom 0.004405 0.000000 0.000000

25 Atom 0.007832 0.000000 0.000000

26 Atom -0.000439 -0.000000 0.000000

27 Atom -0.000957 0.000000 0.000000

28 Atom 0.000132 -0.000000 0.000000

29 Atom 0.005774 0.000000 -0.000000

30 Atom 0.000132 -0.000000 -0.000000

31 Atom 0.005774 0.000000 0.000000

32 Atom -0.000439 -0.000000 -0.000000

33 Atom -0.000957 0.000000 -0.000000

34 Atom -0.001066 0.000000 -0.000000

35 Atom 0.000292 -0.001292 -0.000191

36 Atom 0.000292 0.001292 0.000191

37 Atom -0.000286 0.000168 -0.000540

38 Atom -0.000286 -0.000168 0.000540

39 Atom 0.000024 0.000000 0.000000

40 Atom -0.000286 -0.000168 0.000540

41 Atom -0.000286 0.000168 -0.000540

42 Atom 0.000024 0.000000 -0.000000

43 Atom 0.000292 0.001292 0.000191

44 Atom 0.000292 -0.001292 -0.000191

45 Atom -0.001066 0.000000 -0.000000

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

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

Anisotropic Spin Dipole Couplings in Principal Axis System

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

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

Baa -0.0888 -11.921 -4.254 -3.977 0.2533 0.9674 -0.0000

1 C(13) Bbb -0.0848 -11.374 -4.059 -3.794 0.9674 -0.2533 0.0000

Bcc 0.1736 23.296 8.312 7.771 0.0000 0.0000 1.0000

Baa -0.0232 -0.896 -0.320 -0.299 0.7665 -0.6423 -0.0000

2 N(14) Bbb -0.0197 -0.761 -0.272 -0.254 0.6423 0.7665 -0.0000

Bcc 0.0430 1.657 0.591 0.553 0.0000 0.0000 1.0000

Baa -0.0092 -1.236 -0.441 -0.412 0.0000 0.0000 1.0000

3 C(13) Bbb -0.0033 -0.439 -0.157 -0.146 0.9947 -0.1032 0.0000

Bcc 0.0125 1.675 0.598 0.559 0.1032 0.9947 -0.0000

Baa -0.0646 -8.664 -3.092 -2.890 0.3433 0.9392 -0.0000

4 C(13) Bbb -0.0611 -8.201 -2.926 -2.735 0.9392 -0.3433 0.0000

Bcc 0.1257 16.865 6.018 5.625 0.0000 0.0000 1.0000

Baa -0.0257 -3.445 -1.229 -1.149 0.0000 0.0000 1.0000

5 C(13) Bbb 0.0120 1.613 0.575 0.538 0.9875 -0.1576 -0.0000

Bcc 0.0137 1.832 0.654 0.611 0.1576 0.9875 0.0000

Baa -0.2287 -8.822 -3.148 -2.943 0.4583 0.8888 -0.0000

6 N(14) Bbb -0.2284 -8.808 -3.143 -2.938 0.8888 -0.4583 0.0000

Bcc 0.4571 17.630 6.291 5.881 0.0000 0.0000 1.0000

Baa -0.0284 -3.808 -1.359 -1.270 0.0000 0.0000 1.0000

7 C(13) Bbb 0.0060 0.809 0.289 0.270 0.5564 0.8309 -0.0000

Bcc 0.0224 2.999 1.070 1.000 0.8309 -0.5564 0.0000

Baa -0.0421 -1.624 -0.579 -0.542 0.1413 0.9900 -0.0000

8 N(14) Bbb -0.0382 -1.473 -0.526 -0.491 0.9900 -0.1413 0.0000

Bcc 0.0803 3.097 1.105 1.033 0.0000 0.0000 1.0000

Baa -0.0798 -10.707 -3.821 -3.572 0.9297 -0.3684 0.0000

9 C(13) Bbb -0.0763 -10.236 -3.652 -3.414 0.3684 0.9297 -0.0000

Bcc 0.1561 20.943 7.473 6.986 0.0000 0.0000 1.0000

Baa -0.0227 -3.048 -1.088 -1.017 0.0000 0.0000 1.0000

10 C(13) Bbb 0.0108 1.451 0.518 0.484 0.8943 0.4474 -0.0000

Bcc 0.0119 1.596 0.570 0.533 -0.4474 0.8943 0.0000

Baa -0.0459 -6.158 -2.197 -2.054 0.8746 -0.4848 0.0000

11 C(13) Bbb -0.0429 -5.760 -2.055 -1.921 0.4848 0.8746 0.0000

Bcc 0.0888 11.918 4.253 3.976 0.0000 0.0000 1.0000

Baa -0.1162 -4.481 -1.599 -1.495 0.0000 0.0000 1.0000

12 N(14) Bbb 0.0519 2.001 0.714 0.667 -0.3838 0.9234 -0.0000

Bcc 0.0643 2.480 0.885 0.827 0.9234 0.3838 0.0000

Baa -0.0227 -3.048 -1.088 -1.017 0.0000 0.0000 1.0000

13 C(13) Bbb 0.0108 1.451 0.518 0.484 0.8943 0.4474 0.0000

Bcc 0.0119 1.596 0.570 0.533 -0.4474 0.8943 -0.0000

Baa -0.0459 -6.158 -2.197 -2.054 0.8746 -0.4848 -0.0000

14 C(13) Bbb -0.0429 -5.760 -2.055 -1.921 0.4848 0.8746 -0.0000

Bcc 0.0888 11.918 4.253 3.976 0.0000 0.0000 1.0000

Baa -0.0284 -3.808 -1.359 -1.270 0.0000 0.0000 1.0000

15 C(13) Bbb 0.0060 0.809 0.289 0.270 0.5564 0.8309 -0.0000

Bcc 0.0224 2.999 1.070 1.000 0.8309 -0.5564 -0.0000

Baa -0.0421 -1.624 -0.579 -0.542 0.1413 0.9900 -0.0000

16 N(14) Bbb -0.0382 -1.473 -0.526 -0.491 0.9900 -0.1413 0.0000

Bcc 0.0803 3.097 1.105 1.033 0.0000 0.0000 1.0000

Baa -0.0798 -10.707 -3.821 -3.572 0.9297 -0.3684 -0.0000

17 C(13) Bbb -0.0763 -10.236 -3.652 -3.414 0.3684 0.9297 -0.0000

Bcc 0.1561 20.943 7.473 6.986 0.0000 0.0000 1.0000

Baa -0.2287 -8.822 -3.148 -2.943 0.4583 0.8888 -0.0000

18 N(14) Bbb -0.2284 -8.808 -3.143 -2.938 0.8888 -0.4583 -0.0000

Bcc 0.4571 17.630 6.291 5.881 0.0000 0.0000 1.0000

Baa -0.0232 -0.896 -0.320 -0.299 0.7665 -0.6423 -0.0000

19 N(14) Bbb -0.0197 -0.761 -0.272 -0.254 0.6423 0.7665 -0.0000

Bcc 0.0430 1.657 0.591 0.553 0.0000 0.0000 1.0000

Baa -0.0092 -1.236 -0.441 -0.412 0.0000 0.0000 1.0000

20 C(13) Bbb -0.0033 -0.439 -0.157 -0.146 0.9947 -0.1032 0.0000

Bcc 0.0125 1.675 0.598 0.559 0.1032 0.9947 -0.0000

Baa -0.0646 -8.664 -3.092 -2.890 0.3433 0.9392 -0.0000

21 C(13) Bbb -0.0611 -8.201 -2.926 -2.735 0.9392 -0.3433 0.0000

Bcc 0.1257 16.865 6.018 5.625 0.0000 0.0000 1.0000

Baa -0.0257 -3.445 -1.229 -1.149 0.0000 0.0000 1.0000

22 C(13) Bbb 0.0120 1.613 0.575 0.538 0.9875 -0.1576 0.0000

Bcc 0.0137 1.832 0.654 0.611 0.1576 0.9875 -0.0000

Baa -0.0888 -11.921 -4.254 -3.977 0.2533 0.9674 -0.0000

23 C(13) Bbb -0.0848 -11.374 -4.059 -3.794 0.9674 -0.2533 0.0000

Bcc 0.1736 23.296 8.312 7.771 0.0000 0.0000 1.0000

Baa -0.1162 -4.481 -1.599 -1.495 0.0000 0.0000 1.0000

24 N(14) Bbb 0.0519 2.001 0.714 0.667 -0.3838 0.9234 -0.0000

Bcc 0.0643 2.480 0.885 0.827 0.9234 0.3838 -0.0000

Baa -0.0102 -0.342 -0.122 -0.114 -0.5035 0.8640 -0.0000

25 Zn(67) Bbb 0.0024 0.081 0.029 0.027 0.0000 0.0000 1.0000

Bcc 0.0078 0.260 0.093 0.087 0.8640 0.5035 -0.0000

Baa -0.0018 -0.241 -0.086 -0.080 0.0959 0.9954 -0.0000

26 C(13) Bbb -0.0010 -0.135 -0.048 -0.045 0.0000 0.0000 1.0000

Bcc 0.0028 0.376 0.134 0.126 0.9954 -0.0959 -0.0000

Baa -0.0019 -1.008 -0.360 -0.336 0.0000 0.0000 1.0000

27 H(1) Bbb -0.0005 -0.263 -0.094 -0.088 0.3565 0.9343 0.0000

Bcc 0.0024 1.270 0.453 0.424 0.9343 -0.3565 0.0000

Baa -0.0010 -0.138 -0.049 -0.046 0.9987 -0.0505 0.0000

28 C(13) Bbb -0.0006 -0.075 -0.027 -0.025 -0.0000 -0.0000 1.0000

Bcc 0.0016 0.214 0.076 0.071 0.0505 0.9987 0.0000

Baa -0.0050 -2.676 -0.955 -0.893 -0.6333 0.7739 -0.0000

29 H(1) Bbb -0.0018 -0.935 -0.334 -0.312 0.0000 0.0000 1.0000

Bcc 0.0068 3.611 1.288 1.204 0.7739 0.6333 -0.0000

Baa -0.0010 -0.138 -0.049 -0.046 0.9987 -0.0505 -0.0000

30 C(13) Bbb -0.0006 -0.075 -0.027 -0.025 0.0000 0.0000 1.0000

Bcc 0.0016 0.214 0.076 0.071 0.0505 0.9987 -0.0000

Baa -0.0050 -2.676 -0.955 -0.893 -0.6333 0.7739 0.0000

31 H(1) Bbb -0.0018 -0.935 -0.334 -0.312 0.0000 0.0000 1.0000

Bcc 0.0068 3.611 1.288 1.204 0.7739 0.6333 -0.0000

Baa -0.0018 -0.241 -0.086 -0.080 0.0959 0.9954 -0.0000

32 C(13) Bbb -0.0010 -0.135 -0.048 -0.045 0.0000 0.0000 1.0000

Bcc 0.0028 0.376 0.134 0.126 0.9954 -0.0959 -0.0000

Baa -0.0019 -1.008 -0.360 -0.336 -0.0000 0.0000 1.0000

33 H(1) Bbb -0.0005 -0.263 -0.094 -0.088 0.3565 0.9343 -0.0000

Bcc 0.0024 1.270 0.453 0.424 0.9343 -0.3565 0.0000

Baa -0.0013 -0.702 -0.251 -0.234 0.2858 0.9583 0.0000

34 H(1) Bbb -0.0013 -0.673 -0.240 -0.224 -0.0000 -0.0000 1.0000

Bcc 0.0026 1.375 0.491 0.459 0.9583 -0.2858 0.0000

Baa -0.0020 -1.050 -0.375 -0.350 0.2690 0.1013 0.9578

35 H(1) Bbb -0.0010 -0.510 -0.182 -0.170 -0.1105 0.9911 -0.0738

Bcc 0.0029 1.560 0.557 0.520 0.9568 0.0860 -0.2778

Baa -0.0020 -1.050 -0.375 -0.350 -0.2690 -0.1013 0.9578

36 H(1) Bbb -0.0010 -0.510 -0.182 -0.170 -0.1105 0.9911 0.0738

Bcc 0.0029 1.560 0.557 0.520 0.9568 0.0860 0.2778

Baa -0.0010 -0.550 -0.196 -0.183 -0.2660 0.1723 0.9485

37 H(1) Bbb -0.0006 -0.337 -0.120 -0.112 0.9542 0.1870 0.2336

Bcc 0.0017 0.887 0.316 0.296 -0.1371 0.9671 -0.2141

Baa -0.0010 -0.550 -0.196 -0.183 0.2660 -0.1723 0.9485

38 H(1) Bbb -0.0006 -0.337 -0.120 -0.112 0.9542 0.1870 -0.2336

Bcc 0.0017 0.887 0.316 0.296 -0.1371 0.9671 0.2141

Baa -0.0009 -0.458 -0.163 -0.153 0.0000 0.0000 1.0000

39 H(1) Bbb -0.0004 -0.229 -0.082 -0.076 0.9999 -0.0138 -0.0000

Bcc 0.0013 0.687 0.245 0.229 0.0138 0.9999 -0.0000

Baa -0.0010 -0.550 -0.196 -0.183 0.2660 -0.1723 0.9485

40 H(1) Bbb -0.0006 -0.337 -0.120 -0.112 0.9542 0.1870 -0.2336

Bcc 0.0017 0.887 0.316 0.296 -0.1371 0.9671 0.2141

Baa -0.0010 -0.550 -0.196 -0.183 -0.2660 0.1723 0.9485

41 H(1) Bbb -0.0006 -0.337 -0.120 -0.112 0.9542 0.1870 0.2336

Bcc 0.0017 0.887 0.316 0.296 -0.1371 0.9671 -0.2141

Baa -0.0009 -0.458 -0.163 -0.153 0.0000 0.0000 1.0000

42 H(1) Bbb -0.0004 -0.229 -0.082 -0.076 0.9999 -0.0138 0.0000

Bcc 0.0013 0.687 0.245 0.229 0.0138 0.9999 -0.0000

Baa -0.0020 -1.050 -0.375 -0.350 -0.2690 -0.1013 0.9578

43 H(1) Bbb -0.0010 -0.510 -0.182 -0.170 -0.1105 0.9911 0.0738

Bcc 0.0029 1.560 0.557 0.520 0.9568 0.0860 0.2778

Baa -0.0020 -1.050 -0.375 -0.350 0.2690 0.1013 0.9578

44 H(1) Bbb -0.0010 -0.510 -0.182 -0.170 -0.1105 0.9911 -0.0738

Bcc 0.0029 1.560 0.557 0.520 0.9568 0.0860 -0.2778

Baa -0.0013 -0.702 -0.251 -0.234 0.2858 0.9583 0.0000

45 H(1) Bbb -0.0013 -0.673 -0.240 -0.224 0.0000 0.0000 1.0000

Bcc 0.0026 1.375 0.491 0.459 0.9583 -0.2858 0.0000

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

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Tue Sep 17 13:50:32 2019, MaxMem= 2415919104 cpu: 29.9

(Enter /home/blab/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

Density matrix has only Abelian symmetry.

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

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15315 LenP2D= 41224.

LDataN: DoStor=T MaxTD1= 6 Len= 172

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

GePol: Maximum number of non-zero 1st derivatives = 254

Leave Link 701 at Tue Sep 17 13:50:36 2019, MaxMem= 2415919104 cpu: 79.6

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 13:50:36 2019, MaxMem= 2415919104 cpu: 0.3

(Enter /home/blab/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Density matrix has only Abelian symmetry.

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

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

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

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

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Tue Sep 17 13:50:47 2019, MaxMem= 2415919104 cpu: 195.3

(Enter /home/blab/g09/l716.exe)

Dipole =-7.63833441D-14 1.75859327D-13-2.22044605D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.014835836 -0.006722284 0.000000000

2 7 0.008775346 -0.006678385 0.000000000

3 6 -0.007942273 0.001519430 -0.000000000

4 6 0.005443178 0.006362247 -0.000000000

5 6 -0.001366945 0.009692807 -0.000000000

6 7 0.006478907 -0.008520584 0.000000000

7 6 -0.000809233 0.004635183 -0.000000000

8 7 -0.002868312 -0.012858436 -0.000000000

9 6 0.015459843 0.008478822 -0.000000000

10 6 -0.007347343 0.007122768 -0.000000000

11 6 -0.004222475 0.000371414 -0.000000000

12 7 0.000818138 0.003573795 -0.000000000

13 6 0.007347343 -0.007122768 0.000000000

14 6 0.004222475 -0.000371414 0.000000000

15 6 0.000809233 -0.004635183 -0.000000000

16 7 0.002868312 0.012858436 0.000000000

17 6 -0.015459843 -0.008478822 0.000000000

18 7 -0.006478907 0.008520584 0.000000000

19 7 -0.008775346 0.006678385 0.000000000

20 6 0.007942273 -0.001519430 -0.000000000

21 6 -0.005443178 -0.006362247 0.000000000

22 6 0.001366945 -0.009692807 0.000000000

23 6 0.014835836 0.006722284 0.000000000

24 7 -0.000818138 -0.003573795 -0.000000000

25 30 0.000000000 -0.000000000 -0.000000000

26 6 0.001828855 0.000854716 -0.000000000

27 1 0.000095321 0.000211222 0.000000000

28 6 -0.000072567 0.001378977 0.000000000

29 1 -0.000378833 0.000198603 0.000000000

30 6 0.000072567 -0.001378977 0.000000000

31 1 0.000378833 -0.000198603 0.000000000

32 6 -0.001828855 -0.000854716 0.000000000

33 1 -0.000095321 -0.000211222 -0.000000000

34 1 0.001223918 -0.000312037 -0.000000000

35 1 -0.000956202 -0.000647977 -0.002900313

36 1 -0.000956202 -0.000647977 0.002900313

37 1 0.000331524 -0.001256539 -0.003096833

38 1 0.000331524 -0.001256539 0.003096833

39 1 0.000260519 0.001278892 -0.000000000

40 1 -0.000331524 0.001256539 -0.003096833

41 1 -0.000331524 0.001256539 0.003096833

42 1 -0.000260519 -0.001278892 0.000000000

43 1 0.000956202 0.000647977 -0.002900313

44 1 0.000956202 0.000647977 0.002900313

45 1 -0.001223918 0.000312037 -0.000000000

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

Cartesian Forces: Max 0.015459843 RMS 0.004598045

Leave Link 716 at Tue Sep 17 13:50:47 2019, MaxMem= 2415919104 cpu: 0.4

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

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

Internal Forces: Max 0.011153024 RMS 0.002325181

Search for a local minimum.

Step number 1 out of a maximum of 270

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

Swapping is turned off.

Second derivative matrix not updated -- first step.

ITU= 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01333

Eigenvalues --- 0.01336 0.01336 0.01336 0.01604 0.01623

Eigenvalues --- 0.01636 0.01636 0.01772 0.01788 0.01811

Eigenvalues --- 0.01811 0.01885 0.01901 0.01940 0.01940

Eigenvalues --- 0.01997 0.01998 0.02045 0.02045 0.02070

Eigenvalues --- 0.02086 0.02100 0.02111 0.02111 0.02205

Eigenvalues --- 0.02317 0.02317 0.02353 0.02374 0.07287

Eigenvalues --- 0.07287 0.07287 0.07287 0.07341 0.07341

Eigenvalues --- 0.07341 0.07341 0.14497 0.14497 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 --- 0.16499 0.18264 0.22088 0.22088 0.23816

Eigenvalues --- 0.23854 0.23854 0.23879 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 0.33191 0.33191 0.33222 0.33234

Eigenvalues --- 0.33282 0.33282 0.33282 0.33282 0.33724

Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33724 0.34437 0.34437 0.34437

Eigenvalues --- 0.34437 0.35364 0.35417 0.35563 0.35563

Eigenvalues --- 0.35682 0.35682 0.35682 0.35682 0.39288

Eigenvalues --- 0.41735 0.41735 0.42785 0.47883 0.48973

Eigenvalues --- 0.48973 0.49843 0.50268 0.50571 0.51360

Eigenvalues --- 0.51360 0.51797 0.53989 0.53989 0.54934

Eigenvalues --- 0.56287 0.56340 0.56340 0.56414

Angle between quadratic step and forces= 21.24 degrees.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.00857230 RMS(Int)= 0.00003398

Iteration 2 RMS(Cart)= 0.00007373 RMS(Int)= 0.00001543

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001543

ITry= 1 IFail=0 DXMaxC= 3.22D-02 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

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

(Linear) (Quad) (Total)

R1 2.57723 0.00981 0.00000 0.01939 0.01936 2.59659

R2 2.76294 -0.00910 0.00000 -0.02419 -0.02417 2.73877

R3 2.53844 -0.00228 0.00000 -0.00364 -0.00363 2.53482

R4 2.57400 -0.00295 0.00000 -0.00545 -0.00548 2.56852

R5 3.79361 0.00214 0.00000 0.01233 0.01230 3.80591

R6 2.79211 -0.00671 0.00000 -0.02009 -0.02009 2.77202

R7 2.53307 0.00657 0.00000 0.01223 0.01226 2.54533

R8 2.58757 0.00426 0.00000 0.00809 0.00813 2.59570

R9 2.81859 0.00108 0.00000 0.00324 0.00324 2.82183

R10 2.04583 -0.00020 0.00000 -0.00055 -0.00055 2.04528

R11 2.53844 0.00332 0.00000 0.00650 0.00653 2.54497

R12 2.57723 -0.00359 0.00000 -0.00688 -0.00689 2.57034

R13 2.76294 -0.00275 0.00000 -0.00844 -0.00844 2.75450

R14 2.57400 0.01115 0.00000 0.02194 0.02193 2.59593

R15 3.79361 0.00212 0.00000 0.01145 0.01142 3.80504

R16 2.79211 -0.00993 0.00000 -0.02782 -0.02781 2.76430

R17 2.53307 -0.00508 0.00000 -0.00852 -0.00851 2.52456

R18 2.58757 0.00276 0.00000 0.00498 0.00501 2.59258

R19 2.81859 0.00088 0.00000 0.00265 0.00265 2.82124

R20 2.04583 -0.00037 0.00000 -0.00103 -0.00103 2.04479

R21 2.53307 -0.00508 0.00000 -0.00852 -0.00851 2.52456

R22 2.58757 0.00276 0.00000 0.00498 0.00501 2.59258

R23 2.79211 -0.00993 0.00000 -0.02782 -0.02781 2.76430

R24 2.81859 0.00088 0.00000 0.00265 0.00265 2.82124

R25 2.76294 -0.00275 0.00000 -0.00844 -0.00844 2.75450

R26 2.04583 -0.00037 0.00000 -0.00103 -0.00103 2.04479

R27 2.57723 -0.00359 0.00000 -0.00688 -0.00689 2.57034

R28 2.53844 0.00332 0.00000 0.00650 0.00653 2.54497

R29 2.57400 0.01115 0.00000 0.02194 0.02193 2.59593

R30 3.79361 0.00212 0.00000 0.01145 0.01142 3.80504

R31 2.53307 0.00657 0.00000 0.01223 0.01226 2.54533

R32 2.57400 -0.00295 0.00000 -0.00545 -0.00548 2.56852

R33 2.57723 0.00981 0.00000 0.01939 0.01936 2.59659

R34 3.79361 0.00214 0.00000 0.01233 0.01230 3.80591

R35 2.79211 -0.00671 0.00000 -0.02009 -0.02009 2.77202

R36 2.58757 0.00426 0.00000 0.00809 0.00813 2.59570

R37 2.81859 0.00108 0.00000 0.00324 0.00324 2.82183

R38 2.76294 -0.00910 0.00000 -0.02419 -0.02417 2.73877

R39 2.04583 -0.00020 0.00000 -0.00055 -0.00055 2.04528

R40 2.53844 -0.00228 0.00000 -0.00364 -0.00363 2.53482

R41 2.06599 -0.00079 0.00000 -0.00229 -0.00229 2.06370

R42 2.07798 -0.00272 0.00000 -0.00808 -0.00808 2.06990

R43 2.07798 -0.00272 0.00000 -0.00808 -0.00808 2.06990

R44 2.07798 -0.00311 0.00000 -0.00924 -0.00924 2.06874

R45 2.07798 -0.00311 0.00000 -0.00924 -0.00924 2.06874

R46 2.06599 -0.00086 0.00000 -0.00251 -0.00251 2.06348

R47 2.07798 -0.00311 0.00000 -0.00924 -0.00924 2.06874

R48 2.07798 -0.00311 0.00000 -0.00924 -0.00924 2.06874

R49 2.06599 -0.00086 0.00000 -0.00251 -0.00251 2.06348

R50 2.07798 -0.00272 0.00000 -0.00808 -0.00808 2.06990

R51 2.07798 -0.00272 0.00000 -0.00808 -0.00808 2.06990

R52 2.06599 -0.00079 0.00000 -0.00229 -0.00229 2.06370

A1 1.89137 -0.00322 0.00000 -0.01150 -0.01151 1.87987

A2 2.21236 0.00145 0.00000 0.00516 0.00514 2.21750

A3 2.17945 0.00177 0.00000 0.00634 0.00637 2.18582

A4 1.90638 0.00188 0.00000 0.00975 0.00973 1.91611

A5 2.19032 -0.00117 0.00000 -0.00549 -0.00548 2.18484

A6 2.18649 -0.00071 0.00000 -0.00425 -0.00426 2.18223

A7 1.89647 -0.00193 0.00000 -0.00975 -0.00980 1.88667

A8 2.21943 0.00296 0.00000 0.01349 0.01350 2.23293

A9 2.16729 -0.00103 0.00000 -0.00374 -0.00370 2.16359

A10 1.85108 0.00258 0.00000 0.00841 0.00843 1.85950

A11 2.17776 -0.00251 0.00000 -0.00909 -0.00910 2.16866

A12 2.25435 -0.00007 0.00000 0.00068 0.00067 2.25502

A13 1.87948 0.00069 0.00000 0.00310 0.00314 1.88262

A14 2.17828 -0.00047 0.00000 -0.00232 -0.00234 2.17594

A15 2.22542 -0.00022 0.00000 -0.00079 -0.00081 2.22462

A16 2.18698 -0.00511 0.00000 -0.01778 -0.01776 2.16922

A17 2.21236 0.00254 0.00000 0.01118 0.01119 2.22355

A18 2.17945 0.00008 0.00000 0.00129 0.00130 2.18076

A19 1.89137 -0.00262 0.00000 -0.01247 -0.01249 1.87888

A20 1.90638 0.00137 0.00000 0.00837 0.00836 1.91474

A21 2.19032 0.00044 0.00000 -0.00060 -0.00061 2.18971

A22 2.18649 -0.00181 0.00000 -0.00776 -0.00775 2.17873

A23 1.89647 -0.00219 0.00000 -0.00732 -0.00734 1.88913

A24 2.21943 0.00221 0.00000 0.00806 0.00806 2.22749

A25 2.16729 -0.00002 0.00000 -0.00074 -0.00072 2.16657

A26 1.85108 0.00074 0.00000 0.00227 0.00229 1.85337

A27 2.17776 -0.00044 0.00000 -0.00142 -0.00143 2.17633

A28 2.25435 -0.00030 0.00000 -0.00085 -0.00087 2.25348

A29 1.87948 0.00270 0.00000 0.00915 0.00918 1.88865

A30 2.17828 -0.00157 0.00000 -0.00594 -0.00595 2.17234

A31 2.22542 -0.00113 0.00000 -0.00322 -0.00323 2.22220

A32 2.18698 -0.00079 0.00000 -0.00200 -0.00203 2.18495

A33 1.85108 0.00074 0.00000 0.00227 0.00229 1.85337

A34 2.25435 -0.00030 0.00000 -0.00085 -0.00087 2.25348

A35 2.17776 -0.00044 0.00000 -0.00142 -0.00143 2.17633

A36 1.87948 0.00270 0.00000 0.00915 0.00918 1.88865

A37 2.22542 -0.00113 0.00000 -0.00322 -0.00323 2.22220

A38 2.17828 -0.00157 0.00000 -0.00594 -0.00595 2.17234

A39 1.89137 -0.00262 0.00000 -0.01247 -0.01249 1.87888

A40 2.17945 0.00008 0.00000 0.00129 0.00130 2.18076

A41 2.21236 0.00254 0.00000 0.01118 0.01119 2.22355

A42 1.90638 0.00137 0.00000 0.00837 0.00836 1.91474

A43 2.19032 0.00044 0.00000 -0.00060 -0.00061 2.18971

A44 2.18649 -0.00181 0.00000 -0.00776 -0.00775 2.17873

A45 2.16729 -0.00002 0.00000 -0.00074 -0.00072 2.16657

A46 2.21943 0.00221 0.00000 0.00806 0.00806 2.22749

A47 1.89647 -0.00219 0.00000 -0.00732 -0.00734 1.88913

A48 2.18698 -0.00511 0.00000 -0.01778 -0.01776 2.16922

A49 1.90638 0.00188 0.00000 0.00975 0.00973 1.91611

A50 2.18649 -0.00071 0.00000 -0.00425 -0.00426 2.18223

A51 2.19032 -0.00117 0.00000 -0.00549 -0.00548 2.18484

A52 2.21943 0.00296 0.00000 0.01349 0.01350 2.23293

A53 2.16729 -0.00103 0.00000 -0.00374 -0.00370 2.16359

A54 1.89647 -0.00193 0.00000 -0.00975 -0.00980 1.88667

A55 1.85108 0.00258 0.00000 0.00841 0.00843 1.85950

A56 2.17776 -0.00251 0.00000 -0.00909 -0.00910 2.16866

A57 2.25435 -0.00007 0.00000 0.00068 0.00067 2.25502

A58 1.87948 0.00069 0.00000 0.00310 0.00314 1.88262

A59 2.22542 -0.00022 0.00000 -0.00079 -0.00081 2.22462

A60 2.17828 -0.00047 0.00000 -0.00232 -0.00234 2.17594

A61 1.89137 -0.00322 0.00000 -0.01150 -0.01151 1.87987

A62 2.21236 0.00145 0.00000 0.00516 0.00514 2.21750

A63 2.17945 0.00177 0.00000 0.00634 0.00637 2.18582

A64 2.18698 -0.00079 0.00000 -0.00200 -0.00203 2.18495

A65 1.57080 -0.00011 0.00000 -0.00203 -0.00206 1.56873

A66 1.57080 0.00011 0.00000 0.00203 0.00206 1.57286

A67 1.57080 0.00011 0.00000 0.00203 0.00206 1.57286

A68 1.57080 -0.00011 0.00000 -0.00203 -0.00206 1.56873

A69 1.93538 0.00095 0.00000 0.00696 0.00693 1.94230

A70 1.93656 0.00142 0.00000 0.00835 0.00833 1.94489

A71 1.93656 0.00142 0.00000 0.00835 0.00833 1.94489

A72 1.89112 -0.00108 0.00000 -0.00575 -0.00579 1.88533

A73 1.89112 -0.00108 0.00000 -0.00575 -0.00579 1.88533

A74 1.87099 -0.00182 0.00000 -0.01343 -0.01344 1.85755

A75 1.93656 0.00109 0.00000 0.00628 0.00626 1.94282

A76 1.93656 0.00109 0.00000 0.00628 0.00626 1.94282

A77 1.93538 0.00106 0.00000 0.00774 0.00771 1.94309

A78 1.87099 -0.00150 0.00000 -0.01155 -0.01155 1.85944

A79 1.89112 -0.00096 0.00000 -0.00493 -0.00497 1.88615

A80 1.89112 -0.00096 0.00000 -0.00493 -0.00497 1.88615

A81 1.93656 0.00109 0.00000 0.00628 0.00626 1.94282

A82 1.93656 0.00109 0.00000 0.00628 0.00626 1.94282

A83 1.93538 0.00106 0.00000 0.00774 0.00771 1.94309

A84 1.87099 -0.00150 0.00000 -0.01155 -0.01155 1.85944

A85 1.89112 -0.00096 0.00000 -0.00493 -0.00497 1.88615

A86 1.89112 -0.00096 0.00000 -0.00493 -0.00497 1.88615

A87 1.93656 0.00142 0.00000 0.00835 0.00833 1.94489

A88 1.93656 0.00142 0.00000 0.00835 0.00833 1.94489

A89 1.93538 0.00095 0.00000 0.00696 0.00693 1.94230

A90 1.87099 -0.00182 0.00000 -0.01343 -0.01344 1.85755

A91 1.89112 -0.00108 0.00000 -0.00575 -0.00579 1.88533

A92 1.89112 -0.00108 0.00000 -0.00575 -0.00579 1.88533

A93 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

A94 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

A95 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

A96 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D1 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D2 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D3 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D4 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D5 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D6 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D7 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D8 0.00000 -0.00000 0.00000 0.00000 -0.00000 0.00000

D9 0.00000 0.00000 0.00000 0.00000 -0.00000 0.00000

D10 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D11 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D12 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D13 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D14 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D15 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D16 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D17 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D18 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D19 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D20 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D21 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D22 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D23 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D24 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D25 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D26 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D27 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D28 0.00000 0.00000 0.00000 0.00000 -0.00000 0.00000

D29 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D30 1.03902 -0.00022 0.00000 -0.00298 -0.00299 1.03604

D31 -1.03902 0.00022 0.00000 0.00298 0.00299 -1.03604

D32 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D33 -2.10257 -0.00022 0.00000 -0.00298 -0.00299 -2.10556

D34 2.10257 0.00022 0.00000 0.00298 0.00299 2.10556

D35 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D36 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D37 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D38 0.00000 0.00000 0.00000 0.00000 -0.00000 0.00000

D39 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D40 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D41 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D42 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D43 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D44 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D45 0.00000 -0.00000 0.00000 0.00000 -0.00000 0.00000

D46 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D47 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D48 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D49 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D50 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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D53 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D54 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D55 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D56 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D57 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D58 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D59 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D60 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D61 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D62 0.00000 0.00000 0.00000 0.00000 -0.00000 0.00000

D63 1.03902 -0.00023 0.00000 -0.00315 -0.00316 1.03586

D64 -1.03902 0.00023 0.00000 0.00315 0.00316 -1.03586

D65 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D66 -2.10257 -0.00023 0.00000 -0.00315 -0.00316 -2.10573

D67 2.10257 0.00023 0.00000 0.00315 0.00316 2.10573

D68 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D69 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D70 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D71 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D72 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D73 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D74 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D75 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D76 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D77 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D78 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D79 -2.10257 -0.00023 0.00000 -0.00315 -0.00316 -2.10573

D80 2.10257 0.00023 0.00000 0.00315 0.00316 2.10573

D81 0.00000 0.00000 0.00000 -0.00000 -0.00000 0.00000

D82 1.03902 -0.00023 0.00000 -0.00315 -0.00316 1.03586

D83 -1.03902 0.00023 0.00000 0.00315 0.00316 -1.03586

D84 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D85 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D86 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D87 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D88 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D89 0.00000 0.00000 0.00000 0.00000 -0.00000 0.00000

D90 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D91 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D92 0.00000 0.00000 0.00000 0.00000 -0.00000 0.00000

D93 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D94 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D95 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D96 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D97 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D98 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D99 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D100 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D101 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D102 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D103 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D104 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D105 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D106 0.00000 -0.00000 0.00000 0.00000 -0.00000 0.00000

D107 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D108 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D109 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D110 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D111 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D112 0.00000 0.00000 0.00000 0.00000 -0.00000 0.00000

D113 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D114 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D115 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D116 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D117 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D118 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D119 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D120 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D121 0.00000 0.00000 0.00000 0.00000 -0.00000 0.00000

D122 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D123 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D124 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D125 1.03902 -0.00022 0.00000 -0.00298 -0.00299 1.03604

D126 -1.03902 0.00022 0.00000 0.00298 0.00299 -1.03604

D127 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D128 -2.10257 -0.00022 0.00000 -0.00298 -0.00299 -2.10556

D129 2.10257 0.00022 0.00000 0.00298 0.00299 2.10556

D130 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D131 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D132 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D133 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D134 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D135 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D136 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

Item Value Threshold Converged?

Maximum Force 0.011153 0.000450 NO

RMS Force 0.002325 0.000300 NO

Maximum Displacement 0.032202 0.001800 NO

RMS Displacement 0.008567 0.001200 NO

Predicted change in Energy=-2.063179D-03

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 13:50:48 2019, MaxMem= 2415919104 cpu: 2.7

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.083815 -2.188817 0.000000

2 7 0 -0.747195 -1.870268 0.000000

3 6 0 -0.003141 -3.007730 0.000000

4 6 0 -0.920532 -4.152349 -0.000000

5 6 0 -2.192568 -3.634024 -0.000000

6 7 0 1.339169 -3.119201 0.000000

7 6 0 2.187332 -2.073097 -0.000000

8 7 0 1.868292 -0.750880 0.000000

9 6 0 3.016814 0.002759 -0.000000

10 6 0 4.161798 -0.907627 0.000000

11 6 0 3.641246 -2.176968 0.000000

12 7 0 -3.118222 -1.334846 -0.000000

13 6 0 -4.161798 0.907627 0.000000

14 6 0 -3.641246 2.176968 -0.000000

15 6 0 -2.187332 2.073097 -0.000000

16 7 0 -1.868292 0.750880 0.000000

17 6 0 -3.016814 -0.002759 0.000000

18 7 0 -1.339169 3.119201 0.000000

19 7 0 0.747195 1.870268 0.000000

20 6 0 0.003141 3.007730 -0.000000

21 6 0 0.920532 4.152349 -0.000000

22 6 0 2.192568 3.634024 -0.000000

23 6 0 2.083815 2.188817 -0.000000

24 7 0 3.118222 1.334846 0.000000

25 30 0 0.000000 -0.000000 -0.000000

26 6 0 -0.483119 -5.580094 0.000000

27 1 0 -3.126375 -4.181207 -0.000000

28 6 0 5.590888 -0.475703 0.000000

29 1 0 4.188465 -3.110456 -0.000000

30 6 0 -5.590888 0.475703 0.000000

31 1 0 -4.188465 3.110456 -0.000000

32 6 0 0.483119 5.580094 -0.000000

33 1 0 3.126375 4.181207 0.000000

34 1 0 -1.339916 -6.257217 -0.000000

35 1 0 0.130957 -5.810593 0.877245

36 1 0 0.130957 -5.810593 -0.877245

37 1 0 5.821395 0.137092 0.877374

38 1 0 5.821395 0.137092 -0.877374

39 1 0 6.265369 -1.334435 0.000000

40 1 0 -5.821395 -0.137092 0.877374

41 1 0 -5.821395 -0.137092 -0.877374

42 1 0 -6.265369 1.334435 0.000000

43 1 0 -0.130957 5.810593 0.877245

44 1 0 -0.130957 5.810593 -0.877245

45 1 0 1.339916 6.257217 0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.374055 0.000000

3 C 2.236028 1.359204 0.000000

4 C 2.282254 2.288655 1.466888 0.000000

5 C 1.449293 2.280337 2.277242 1.373585 0.000000

6 N 3.547172 2.431614 1.346931 2.484682 3.569062

7 C 4.272714 2.941528 2.381535 3.739266 4.649733

8 N 4.205569 2.844961 2.931832 4.398583 4.980272

9 C 5.551524 4.204283 4.264173 5.724301 6.353255

10 C 6.375667 5.002489 4.664457 6.029785 6.914565

11 C 5.725073 4.399145 3.737877 4.971111 6.013018

12 N 1.341367 2.430730 3.535855 3.573257 2.478519

13 C 3.729072 4.401842 5.711781 6.009090 4.950198

14 C 4.635264 4.975506 6.333790 6.889307 5.988848

15 C 4.263171 4.198110 5.530416 6.353028 5.707124

16 N 2.947587 2.850838 4.195943 4.993987 4.396878

17 C 2.376834 2.939177 4.255828 4.649032 3.723637

18 N 5.359996 5.024464 6.270905 7.283591 6.806933

19 N 4.948817 4.028004 4.935369 6.249259 6.240147

20 C 5.599954 4.935369 6.015463 7.219412 6.995287

21 C 7.016872 6.249259 7.219412 8.506323 8.385643

22 C 7.224467 6.240147 6.995287 8.385643 8.488459

23 C 6.044238 4.948817 5.599954 7.016872 7.224467

24 N 6.283103 5.021375 5.347979 6.813285 7.272837

25 Zn 3.022119 2.014002 3.007732 4.253162 4.244230

26 C 3.750065 3.719212 2.616760 1.493246 2.590251

27 H 2.248677 3.316766 3.336411 2.206032 1.082315

28 C 7.863575 6.489692 6.140384 7.477721 8.399831

29 H 6.339630 5.089086 4.192865 5.214153 6.402476

30 C 4.404455 5.381909 6.584619 6.575035 5.332770

31 H 5.701916 6.053921 7.412768 7.964152 7.033606

32 C 8.182000 7.551262 8.601579 9.833142 9.594752

33 H 8.229416 7.185047 7.840579 9.264212 9.453517

34 H 4.135851 4.426809 3.513706 2.146241 2.758289

35 H 4.334978 4.131206 2.939997 2.150572 3.302389

36 H 4.334978 4.131206 2.939997 2.150572 3.302389

37 H 8.286856 6.924280 6.677194 8.038823 8.900264

38 H 8.286856 6.924280 6.677194 8.038823 8.900264

39 H 8.392785 7.033006 6.488000 7.718667 8.764976

40 H 4.353030 5.433341 6.546940 6.396135 5.115341

41 H 4.353030 5.433341 6.546940 6.396135 5.115341

42 H 5.467971 6.381252 7.620361 7.659771 6.424430

43 H 8.280928 7.755317 8.862771 10.032607 9.706729

44 H 8.280928 7.755317 8.862771 10.032607 9.706729

45 H 9.113585 8.391189 9.361787 10.652169 10.503099

6 7 8 9 10

6 N 0.000000

7 C 1.346742 0.000000

8 N 2.426709 1.360164 0.000000

9 C 3.544168 2.235446 1.373708 0.000000

10 C 3.585847 2.292780 2.298856 1.462802 0.000000

11 C 2.487441 1.457619 2.275322 2.267405 1.371934

12 N 4.801276 5.356670 5.020592 6.279160 7.292545

13 C 6.817329 7.013998 6.254010 7.235417 8.519237

14 C 7.270071 7.213555 6.239175 7.004067 8.390603

15 C 6.276637 6.027322 4.941957 5.600843 7.013998

16 N 5.026463 4.941957 4.027077 4.942059 6.254010

17 C 5.356006 5.600843 4.942059 6.033631 7.235417

18 N 6.789047 6.276637 5.026463 5.356006 6.817329

19 N 5.024464 4.198110 2.850838 2.939177 4.401842

20 C 6.270905 5.530416 4.195943 4.255828 5.711781

21 C 7.283591 6.353028 4.993987 4.649032 6.009090

22 C 6.806933 5.707124 4.396878 3.723637 4.950198

23 C 5.359996 4.263171 2.947587 2.376834 3.729072

24 N 4.796203 3.532794 2.431579 1.335942 2.473406

25 Zn 3.394523 3.013661 2.013538 3.016815 4.259619

26 C 3.062143 4.407984 5.371260 6.589216 6.588414

27 H 4.590091 5.716608 6.059195 7.432654 7.989606

28 C 5.006515 3.759769 3.732752 2.618163 1.492935

29 H 2.849309 2.254029 3.309199 3.326390 2.202991

30 C 7.806985 8.185174 7.559357 8.620685 9.850304

31 H 8.328467 8.217056 7.182912 7.846899 9.266708

32 C 8.741313 7.840642 6.480735 6.125869 7.458096

33 H 7.515987 6.324407 5.090015 4.179884 5.193104

34 H 4.126092 5.472507 6.372782 7.626821 7.673785

35 H 3.077812 4.355124 5.421124 6.549259 6.407521

36 H 3.077812 4.355124 5.421124 6.549259 6.407521

37 H 5.609241 4.342941 4.145516 2.941684 2.148368

38 H 5.609241 4.342941 4.145516 2.941684 2.148368

39 H 5.239546 4.144395 4.435631 3.513004 2.146433

40 H 7.806180 8.285989 7.763879 8.882752 10.051252

41 H 7.806180 8.285989 7.763879 8.882752 10.051252

42 H 8.812711 9.113695 8.396725 9.377222 10.665490

43 H 9.092417 8.264175 6.915163 6.664005 8.020709

44 H 9.092417 8.264175 6.915163 6.664005 8.020709

45 H 9.376418 8.373306 7.027987 6.475356 7.700520

11 12 13 14 15

11 C 0.000000

12 N 6.811723 0.000000

13 C 8.390603 2.473406 0.000000

14 C 8.484777 3.550549 1.371934 0.000000

15 C 7.213555 3.532794 2.292780 1.457619 0.000000

16 N 6.239175 2.431579 2.298856 2.275322 1.360164

17 C 7.004067 1.335942 1.462802 2.267405 2.235446

18 N 7.270071 4.796203 3.585847 2.487441 1.346742

19 N 4.975506 5.021375 5.002489 4.399145 2.941528

20 C 6.333790 5.347979 4.664457 3.737877 2.381535

21 C 6.889307 6.813285 6.029785 4.971111 3.739266

22 C 5.988848 7.272837 6.914565 6.013018 4.649733

23 C 4.635264 6.283103 6.375667 5.725073 4.272714

24 N 3.550549 6.783840 7.292545 6.811723 5.356670

25 Zn 4.242389 3.391920 4.259619 4.242389 3.013661

26 C 5.347115 4.996588 7.458096 8.375308 7.840642

27 H 7.058163 2.846372 5.193104 6.378988 6.324407

28 C 2.587549 8.751384 9.850304 9.605673 8.185174

29 H 1.082057 7.519339 9.266708 9.447816 8.217056

30 C 9.605673 3.064664 1.492935 2.587549 3.759769

31 H 9.447816 4.572322 2.202991 1.082057 2.254029

32 C 8.375308 7.796540 6.588414 5.347115 4.407984

33 H 6.378988 8.331976 7.989606 7.058163 5.716608

34 H 6.438975 5.233747 7.700520 8.742517 8.373306

35 H 5.127857 5.599913 8.020709 8.876948 8.264175

36 H 5.127857 5.599913 8.020709 8.876948 8.264175

37 H 3.298138 9.102370 10.051252 9.719694 8.285989

38 H 3.298138 9.102370 10.051252 9.719694 8.285989

39 H 2.756064 9.383591 10.665490 10.510517 9.113695

40 H 9.719694 3.084080 2.148368 3.298138 4.342941

41 H 9.719694 3.084080 2.148368 3.298138 4.342941

42 H 10.510517 4.126693 2.146433 2.756064 4.144395

43 H 8.876948 7.794268 6.407521 5.127857 4.355124

44 H 8.876948 7.794268 6.407521 5.127857 4.355124

45 H 8.742517 8.804227 7.673785 6.438975 5.472507

16 17 18 19 20

16 N 0.000000

17 C 1.373708 0.000000

18 N 2.426709 3.544168 0.000000

19 N 2.844961 4.204283 2.431614 0.000000

20 C 2.931832 4.264173 1.346931 1.359204 0.000000

21 C 4.398583 5.724301 2.484682 2.288655 1.466888

22 C 4.980272 6.353255 3.569062 2.280337 2.277242

23 C 4.205569 5.551524 3.547172 1.374055 2.236028

24 N 5.020592 6.279160 4.801276 2.430730 3.535855

25 Zn 2.013538 3.016815 3.394523 2.014002 3.007732

26 C 6.480735 6.125869 8.741313 7.551262 8.601579

27 H 5.090015 4.179884 7.515987 7.185047 7.840579

28 C 7.559357 8.620685 7.806985 5.381909 6.584619

29 H 7.182912 7.846899 8.328467 6.053921 7.412768

30 C 3.732752 2.618163 5.006515 6.489692 6.140384

31 H 3.309199 3.326390 2.849309 5.089086 4.192865

32 C 5.371260 6.589216 3.062143 3.719212 2.616760

33 H 6.059195 7.432654 4.590091 3.316766 3.336411

34 H 7.027987 6.475356 9.376418 8.391189 9.361787

35 H 6.915163 6.664005 9.092417 7.755317 8.862771

36 H 6.915163 6.664005 9.092417 7.755317 8.862771

37 H 7.763879 8.882752 7.806180 5.433341 6.546940

38 H 7.763879 8.882752 7.806180 5.433341 6.546940

39 H 8.396725 9.377222 8.812711 6.381252 7.620361

40 H 4.145516 2.941684 5.609241 6.924280 6.677194

41 H 4.145516 2.941684 5.609241 6.924280 6.677194

42 H 4.435631 3.513004 5.239546 7.033006 6.488000

43 H 5.421124 6.549259 3.077812 4.131206 2.939997

44 H 5.421124 6.549259 3.077812 4.131206 2.939997

45 H 6.372782 7.626821 4.126092 4.426809 3.513706

21 22 23 24 25

21 C 0.000000

22 C 1.373585 0.000000

23 C 2.282254 1.449293 0.000000

24 N 3.573257 2.478519 1.341367 0.000000

25 Zn 4.253162 4.244230 3.022119 3.391920 0.000000

26 C 9.833142 9.594752 8.182000 7.796540 5.600968

27 H 9.264212 9.453517 8.229416 8.331976 5.220796

28 C 6.575035 5.332770 4.404455 3.064664 5.611089

29 H 7.964152 7.033606 5.701916 4.572322 5.217104

30 C 7.477721 8.399831 7.863575 8.751384 5.611089

31 H 5.214153 6.402476 6.339630 7.519339 5.217104

32 C 1.493246 2.590251 3.750065 4.996588 5.600968

33 H 2.206032 1.082315 2.248677 2.846372 5.220796

34 H 10.652169 10.503099 9.113585 8.804227 6.399073

35 H 10.032607 9.706729 8.280928 7.794268 5.877899

36 H 10.032607 9.706729 8.280928 7.794268 5.877899

37 H 6.396135 5.115341 4.353030 3.084080 5.888737

38 H 6.396135 5.115341 4.353030 3.084080 5.888737

39 H 7.659771 6.424430 5.467971 4.126693 6.405901

40 H 8.038823 8.900264 8.286856 9.102370 5.888737

41 H 8.038823 8.900264 8.286856 9.102370 5.888737

42 H 7.718667 8.764976 8.392785 9.383591 6.405901

43 H 2.150572 3.302389 4.334978 5.599913 5.877899

44 H 2.150572 3.302389 4.334978 5.599913 5.877899

45 H 2.146241 2.758289 4.135851 5.233747 6.399073

26 27 28 29 30

26 C 0.000000

27 H 2.990600 0.000000

28 C 7.934000 9.472140 0.000000

29 H 5.284203 7.392793 2.984747 0.000000

30 C 7.922246 5.268836 11.222177 10.416154 0.000000

31 H 9.447499 7.368608 10.416154 10.434208 2.984747

32 C 11.201937 10.407278 7.922246 9.447499 7.934000

33 H 10.407278 10.441592 5.268836 7.368608 9.472140

34 H 1.092061 2.738842 9.025627 6.361218 7.962598

35 H 1.095343 3.746287 7.683844 4.952138 8.545559

36 H 1.095343 3.746287 7.683844 4.952138 8.545559

37 H 8.555869 9.973970 1.094731 3.739360 11.450967

38 H 8.555869 9.973970 1.094731 3.739360 11.450967

39 H 7.972936 9.813714 1.091946 2.732725 11.993641

40 H 7.674194 4.938399 11.450967 10.478930 1.094731

41 H 7.674194 4.938399 11.450967 10.478930 1.094731

42 H 9.013608 6.346305 11.993641 11.359564 1.091946

43 H 11.429843 10.467958 8.545559 9.950481 7.683844

44 H 11.429843 10.467958 8.545559 9.950481 7.683844

45 H 11.976868 11.353786 7.962598 9.791197 9.025627

31 32 33 34 35

31 H 0.000000

32 C 5.284203 0.000000

33 H 7.392793 2.990600 0.000000

34 H 9.791197 11.976868 11.353786 0.000000

35 H 9.950481 11.429843 10.467958 1.769886 0.000000

36 H 9.950481 11.429843 10.467958 1.769886 1.754489

37 H 10.478930 7.674194 4.938399 9.640609 8.231406

38 H 10.478930 7.674194 4.938399 9.640609 8.416337

39 H 11.359564 9.013608 6.346305 9.059478 7.644381

40 H 3.739360 8.555869 9.973970 7.636058 8.223084

41 H 3.739360 8.555869 9.973970 7.636058 8.408198

42 H 2.732725 7.972936 9.813714 9.049490 9.629848

43 H 4.952138 1.095343 3.746287 12.159900 11.624137

44 H 4.952138 1.095343 3.746287 12.159900 11.755798

45 H 6.361218 1.092061 2.738842 12.798147 12.159900

36 37 38 39 40

36 H 0.000000

37 H 8.416337 0.000000

38 H 8.231406 1.754748 0.000000

39 H 7.644381 1.769827 1.769827 0.000000

40 H 8.408198 11.646019 11.777474 12.177574 0.000000

41 H 8.223084 11.777474 11.646019 12.177574 1.754748

42 H 9.629848 12.177574 12.177574 12.811802 1.769827

43 H 11.755798 8.223084 8.408198 9.629848 8.231406

44 H 11.624137 8.408198 8.223084 9.629848 8.416337

45 H 12.159900 7.636058 7.636058 9.049490 9.640609

41 42 43 44 45

41 H 0.000000

42 H 1.769827 0.000000

43 H 8.416337 7.644381 0.000000

44 H 8.231406 7.644381 1.754489 0.000000

45 H 9.640609 9.059478 1.769886 1.769886 0.000000

Stoichiometry C20H16N8Zn(1-,2)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

Omega: Change in point group or standard orientation.

Old FWG=C04H [O(Zn1),SGH(C20H8N8),X(H8)]

New FWG=C02H [O(Zn1),SGH(C20H8N8),X(H8)]

RotChk: IX=3 Diff= 5.37D-01

Largest Abelian subgroup C2H NOp 4

Largest concise Abelian subgroup C2H NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.808014 1.117255 0.000000

2 7 0 -2.013998 -0.004156 0.000000

3 6 0 -2.791940 -1.118715 0.000000

4 6 0 -4.196101 -0.694346 0.000000

5 6 0 -4.189527 0.679223 0.000000

6 7 0 -2.394801 -2.405767 0.000000

7 6 0 -1.107865 -2.802640 0.000000

8 7 0 0.000000 -2.013538 0.000000

9 6 0 1.127577 -2.798168 0.000000

10 6 0 0.709844 -4.200056 0.000000

11 6 0 -0.662056 -4.190411 0.000000

12 7 0 -2.401391 2.395505 0.000000

13 6 0 -0.709844 4.200056 0.000000

14 6 0 0.662056 4.190411 0.000000

15 6 0 1.107865 2.802640 0.000000

16 7 0 0.000000 2.013538 0.000000

17 6 0 -1.127577 2.798168 0.000000

18 7 0 2.394801 2.405767 0.000000

19 7 0 2.013998 0.004156 0.000000

20 6 0 2.791940 1.118715 0.000000

21 6 0 4.196101 0.694346 0.000000

22 6 0 4.189527 -0.679223 0.000000

23 6 0 2.808014 -1.117255 0.000000

24 7 0 2.401391 -2.395505 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -5.357737 -1.632635 0.000000

27 1 0 -5.045471 1.341618 0.000000

28 6 0 1.643541 -5.364987 0.000000

29 1 0 -1.324140 -5.046269 0.000000

30 6 0 -1.643541 5.364987 0.000000

31 1 0 1.324140 5.046269 0.000000

32 6 0 5.357737 1.632635 0.000000

33 1 0 5.045471 -1.341618 0.000000

34 1 0 -6.305530 -1.090152 0.000000

35 1 0 -5.342611 -2.288371 0.877245

36 1 0 -5.342611 -2.288371 -0.877245

37 1 0 2.298092 -5.350347 0.877374

38 1 0 2.298092 -5.350347 -0.877374

39 1 0 1.098278 -6.311050 0.000000

40 1 0 -2.298092 5.350347 0.877374

41 1 0 -2.298092 5.350347 -0.877374

42 1 0 -1.098278 6.311050 0.000000

43 1 0 5.342611 2.288371 0.877245

44 1 0 5.342611 2.288371 -0.877245

45 1 0 6.305530 1.090152 0.000000

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

Rotational constants (GHZ): 0.1826506 0.1817517 0.0913043

Leave Link 202 at Tue Sep 17 13:50:48 2019, MaxMem= 2415919104 cpu: 0.2

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 229 symmetry adapted cartesian basis functions of AG symmetry.

There are 82 symmetry adapted cartesian basis functions of BG symmetry.

There are 78 symmetry adapted cartesian basis functions of AU symmetry.

There are 218 symmetry adapted cartesian basis functions of BU symmetry.

There are 212 symmetry adapted basis functions of AG symmetry.

There are 82 symmetry adapted basis functions of BG symmetry.

There are 78 symmetry adapted basis functions of AU symmetry.

There are 204 symmetry adapted basis functions of BU symmetry.

576 basis functions, 1015 primitive gaussians, 607 cartesian basis functions

103 alpha electrons 102 beta electrons

nuclear repulsion energy 2760.1132594005 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= 45 NActive= 45 NUniq= 21 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1141944131 Hartrees.

Nuclear repulsion after empirical dispersion term = 2759.9990649874 Hartrees.

No density basis found on file 724.

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

Polarizable Continuum Model (PCM)

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

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

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 = 45

GePol: Total number of spheres = 45

GePol: Number of exposed spheres = 45 (100.00%)

GePol: Number of points = 3490

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.10D-10

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 132

GePol: Fraction of low-weight points (<1% of avg) = 3.78%

GePol: Cavity surface area = 382.080 Ang\*\*2

GePol: Cavity volume = 379.159 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0106980312 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2759.9883669562 Hartrees.

Leave Link 301 at Tue Sep 17 13:50:48 2019, MaxMem= 2415919104 cpu: 2.1

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15323 LenP2D= 41234.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.80D-04 NBF= 212 82 78 204

NBsUse= 576 1.00D-06 EigRej= -1.00D+00 NBFU= 212 82 78 204

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= 594 594 594 594 594 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Tue Sep 17 13:50:49 2019, MaxMem= 2415919104 cpu: 20.7

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 13:50:49 2019, MaxMem= 2415919104 cpu: 1.3

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

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

B after Tr= -0.000000 -0.000000 0.000000

Rot= 0.981851 -0.000000 0.000000 -0.189653 Ang= -21.87 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-BG.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7695 S= 0.5097

Generating alternative initial guess.

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -1276.41059133679

Leave Link 401 at Tue Sep 17 13:50:51 2019, MaxMem= 2415919104 cpu: 41.6

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1141655 IEndB= 1141655 NGot= 2415919104 MDV= 2415163146

LenX= 2415163146 LenY= 2414794090

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= 670000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 36540300.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.22D-15 for 3475.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.48D-15 for 2381 433.

Iteration 1 A^-1\*A deviation from unit magnitude is 4.88D-15 for 3475.

Iteration 1 A^-1\*A deviation from orthogonality is 4.16D-14 for 3269 3130.

E= -1276.01205937854

DIIS: error= 9.74D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1276.01205937854 IErMin= 1 ErrMin= 9.74D-04

ErrMax= 9.74D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.33D-03 BMatP= 3.33D-03

IDIUse=3 WtCom= 9.90D-01 WtEn= 9.74D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.287 Goal= None Shift= 0.000

Gap= 0.342 Goal= None Shift= 0.000

RMSDP=9.60D-05 MaxDP=2.11D-03 OVMax= 8.98D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 9.60D-05 CP: 1.00D+00

E= -1276.01300860535 Delta-E= -0.000949226813 Rises=F Damp=F

DIIS: error= 4.82D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1276.01300860535 IErMin= 2 ErrMin= 4.82D-04

ErrMax= 4.82D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.50D-04 BMatP= 3.33D-03

IDIUse=3 WtCom= 9.95D-01 WtEn= 4.82D-03

Coeff-Com: 0.157D+00 0.843D+00

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

Coeff: 0.156D+00 0.844D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=2.92D-05 MaxDP=1.29D-03 DE=-9.49D-04 OVMax= 4.90D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.92D-05 CP: 1.00D+00 9.79D-01

E= -1276.01296321762 Delta-E= 0.000045387736 Rises=F Damp=F

DIIS: error= 6.94D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1276.01300860535 IErMin= 2 ErrMin= 4.82D-04

ErrMax= 6.94D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.71D-04 BMatP= 4.50D-04

IDIUse=3 WtCom= 2.75D-01 WtEn= 7.25D-01

Coeff-Com: -0.422D-02 0.553D+00 0.451D+00

Coeff-En: 0.000D+00 0.583D+00 0.417D+00

Coeff: -0.116D-02 0.575D+00 0.426D+00

Gap= 0.037 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=2.01D-05 MaxDP=7.17D-04 DE= 4.54D-05 OVMax= 3.60D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.17D-05 CP: 1.00D+00 1.02D+00 4.54D-01

E= -1276.01310556064 Delta-E= -0.000142343024 Rises=F Damp=F

DIIS: error= 8.77D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1276.01310556064 IErMin= 4 ErrMin= 8.77D-05

ErrMax= 8.77D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.06D-05 BMatP= 4.50D-04

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

Coeff-Com: -0.815D-02 0.194D+00 0.171D+00 0.643D+00

Coeff: -0.815D-02 0.194D+00 0.171D+00 0.643D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=5.69D-06 MaxDP=1.90D-04 DE=-1.42D-04 OVMax= 3.42D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 5.36D-06 CP: 1.00D+00 1.02D+00 5.13D-01 1.03D+00

E= -1276.01310894076 Delta-E= -0.000003380120 Rises=F Damp=F

DIIS: error= 7.34D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1276.01310894076 IErMin= 5 ErrMin= 7.34D-05

ErrMax= 7.34D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.07D-06 BMatP= 1.06D-05

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

Coeff-Com: -0.437D-02 0.586D-01 0.579D-01 0.385D+00 0.502D+00

Coeff: -0.437D-02 0.586D-01 0.579D-01 0.385D+00 0.502D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=3.66D-06 MaxDP=1.42D-04 DE=-3.38D-06 OVMax= 2.65D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.28D-06 CP: 1.00D+00 1.03D+00 5.25D-01 1.24D+00 1.28D+00

E= -1276.01311095055 Delta-E= -0.000002009785 Rises=F Damp=F

DIIS: error= 7.02D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1276.01311095055 IErMin= 6 ErrMin= 7.02D-05

ErrMax= 7.02D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.99D-07 BMatP= 4.07D-06

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

Coeff-Com: -0.108D-02 0.679D-02 0.109D-01 0.113D+00 0.216D+00 0.655D+00

Coeff: -0.108D-02 0.679D-02 0.109D-01 0.113D+00 0.216D+00 0.655D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=3.93D-06 MaxDP=1.45D-04 DE=-2.01D-06 OVMax= 3.13D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 9.16D-07 CP: 1.00D+00 1.03D+00 5.53D-01 1.43D+00 1.79D+00

CP: 1.49D+00

E= -1276.01311234209 Delta-E= -0.000001391541 Rises=F Damp=F

DIIS: error= 6.57D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1276.01311234209 IErMin= 7 ErrMin= 6.57D-05

ErrMax= 6.57D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.54D-07 BMatP= 4.99D-07

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

Coeff-Com: 0.161D-02-0.288D-01-0.229D-01-0.126D+00-0.129D+00 0.403D+00

Coeff-Com: 0.902D+00

Coeff: 0.161D-02-0.288D-01-0.229D-01-0.126D+00-0.129D+00 0.403D+00

Coeff: 0.902D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=6.63D-06 MaxDP=2.55D-04 DE=-1.39D-06 OVMax= 5.32D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 5.80D-07 CP: 1.00D+00 1.04D+00 5.93D-01 1.75D+00 2.63D+00

CP: 2.60D+00 2.05D+00

E= -1276.01311443837 Delta-E= -0.000002096279 Rises=F Damp=F

DIIS: error= 5.72D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1276.01311443837 IErMin= 8 ErrMin= 5.72D-05

ErrMax= 5.72D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.31D-07 BMatP= 3.54D-07

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

Coeff-Com: 0.103D-02-0.910D-02-0.784D-02-0.959D-01-0.180D+00-0.337D+00

Coeff-Com: 0.215D+00 0.141D+01

Coeff: 0.103D-02-0.910D-02-0.784D-02-0.959D-01-0.180D+00-0.337D+00

Coeff: 0.215D+00 0.141D+01

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=1.05D-05 MaxDP=4.05D-04 DE=-2.10D-06 OVMax= 8.43D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 6.07D-06 CP: 1.00D+00 1.05D+00 6.59D-01 2.26D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.08D+00

E= -1276.01311715329 Delta-E= -0.000002714924 Rises=F Damp=F

DIIS: error= 4.43D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1276.01311715329 IErMin= 9 ErrMin= 4.43D-05

ErrMax= 4.43D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.94D-07 BMatP= 2.31D-07

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

Coeff-Com: -0.619D-03 0.188D-01 0.171D-01 0.333D-01-0.306D-01-0.675D+00

Coeff-Com: -0.647D+00 0.132D+01 0.963D+00

Coeff: -0.619D-03 0.188D-01 0.171D-01 0.333D-01-0.306D-01-0.675D+00

Coeff: -0.647D+00 0.132D+01 0.963D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=1.24D-05 MaxDP=4.80D-04 DE=-2.71D-06 OVMax= 9.98D-03

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.05D-06 CP: 1.00D+00 1.06D+00 7.33D-01 2.86D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.63D+00

E= -1276.01311951125 Delta-E= -0.000002357955 Rises=F Damp=F

DIIS: error= 2.93D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1276.01311951125 IErMin=10 ErrMin= 2.93D-05

ErrMax= 2.93D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.45D-08 BMatP= 1.94D-07

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

Coeff-Com: -0.982D-03 0.122D-01 0.151D-01 0.804D-01 0.146D+00 0.345D-01

Coeff-Com: -0.335D+00-0.681D+00 0.383D+00 0.135D+01

Coeff: -0.982D-03 0.122D-01 0.151D-01 0.804D-01 0.146D+00 0.345D-01

Coeff: -0.335D+00-0.681D+00 0.383D+00 0.135D+01

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=1.11D-05 MaxDP=4.31D-04 DE=-2.36D-06 OVMax= 8.93D-03

Cycle 11 Pass 1 IDiag 1:

RMSU= 8.05D-06 CP: 1.00D+00 1.07D+00 8.04D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 3.00D+00 2.08D+00

E= -1276.01312085545 Delta-E= -0.000001344203 Rises=F Damp=F

DIIS: error= 1.59D-05 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1276.01312085545 IErMin=11 ErrMin= 1.59D-05

ErrMax= 1.59D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.67D-08 BMatP= 9.45D-08

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

Coeff-Com: -0.306D-03-0.303D-02 0.879D-03 0.335D-01 0.113D+00 0.419D+00

Coeff-Com: 0.200D+00-0.124D+01-0.324D+00 0.806D+00 0.999D+00

Coeff: -0.306D-03-0.303D-02 0.879D-03 0.335D-01 0.113D+00 0.419D+00

Coeff: 0.200D+00-0.124D+01-0.324D+00 0.806D+00 0.999D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=7.89D-06 MaxDP=3.06D-04 DE=-1.34D-06 OVMax= 6.33D-03

Cycle 12 Pass 1 IDiag 1:

RMSU= 3.25D-07 CP: 1.00D+00 1.08D+00 8.52D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 3.00D+00 2.98D+00

CP: 1.95D+00

E= -1276.01312136702 Delta-E= -0.000000511570 Rises=F Damp=F

DIIS: error= 7.40D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1276.01312136702 IErMin=12 ErrMin= 7.40D-06

ErrMax= 7.40D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.24D-08 BMatP= 4.67D-08

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

Coeff-Com: 0.298D-03-0.720D-02-0.638D-02-0.203D-01-0.195D-01 0.180D+00

Coeff-Com: 0.250D+00-0.256D+00-0.313D+00-0.280D+00 0.440D+00 0.103D+01

Coeff: 0.298D-03-0.720D-02-0.638D-02-0.203D-01-0.195D-01 0.180D+00

Coeff: 0.250D+00-0.256D+00-0.313D+00-0.280D+00 0.440D+00 0.103D+01

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=4.28D-06 MaxDP=1.67D-04 DE=-5.12D-07 OVMax= 3.44D-03

Cycle 13 Pass 1 IDiag 1:

RMSU= 4.90D-07 CP: 1.00D+00 1.08D+00 8.78D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 2.47D+00 1.47D+00

E= -1276.01312148638 Delta-E= -0.000000119359 Rises=F Damp=F

DIIS: error= 2.25D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1276.01312148638 IErMin=13 ErrMin= 2.25D-06

ErrMax= 2.25D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.84D-09 BMatP= 1.24D-08

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

Coeff-Com: 0.166D-03-0.205D-02-0.239D-02-0.127D-01-0.270D-01-0.785D-02

Coeff-Com: 0.350D-01 0.128D+00-0.581D-01-0.235D+00-0.265D-01 0.375D+00

Coeff-Com: 0.833D+00

Coeff: 0.166D-03-0.205D-02-0.239D-02-0.127D-01-0.270D-01-0.785D-02

Coeff: 0.350D-01 0.128D+00-0.581D-01-0.235D+00-0.265D-01 0.375D+00

Coeff: 0.833D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=1.72D-06 MaxDP=6.60D-05 DE=-1.19D-07 OVMax= 1.38D-03

Cycle 14 Pass 1 IDiag 1:

RMSU= 8.35D-08 CP: 1.00D+00 1.08D+00 8.89D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 2.67D+00 1.70D+00 1.39D+00

E= -1276.01312150099 Delta-E= -0.000000014610 Rises=F Damp=F

DIIS: error= 1.01D-06 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1276.01312150099 IErMin=14 ErrMin= 1.01D-06

ErrMax= 1.01D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.32D-09 BMatP= 2.84D-09

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

Coeff-Com: 0.139D-04 0.945D-03 0.575D-03-0.254D-02-0.121D-01-0.626D-01

Coeff-Com: -0.546D-01 0.172D+00 0.662D-01-0.647D-01-0.162D+00-0.730D-01

Coeff-Com: 0.524D+00 0.668D+00

Coeff: 0.139D-04 0.945D-03 0.575D-03-0.254D-02-0.121D-01-0.626D-01

Coeff: -0.546D-01 0.172D+00 0.662D-01-0.647D-01-0.162D+00-0.730D-01

Coeff: 0.524D+00 0.668D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=1.62D-07 MaxDP=6.33D-06 DE=-1.46D-08 OVMax= 1.26D-04

Cycle 15 Pass 1 IDiag 1:

RMSU= 4.08D-08 CP: 1.00D+00 1.08D+00 8.90D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 2.69D+00 1.74D+00 1.46D+00 8.45D-01

E= -1276.01312150191 Delta-E= -0.000000000922 Rises=F Damp=F

DIIS: error= 4.93D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1276.01312150191 IErMin=15 ErrMin= 4.93D-07

ErrMax= 4.93D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.10D-10 BMatP= 1.32D-09

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

Coeff-Com: -0.318D-04 0.932D-03 0.886D-03 0.156D-02 0.462D-03-0.291D-01

Coeff-Com: -0.339D-01 0.494D-01 0.441D-01 0.186D-01-0.717D-01-0.108D+00

Coeff-Com: 0.455D-01 0.313D+00 0.769D+00

Coeff: -0.318D-04 0.932D-03 0.886D-03 0.156D-02 0.462D-03-0.291D-01

Coeff: -0.339D-01 0.494D-01 0.441D-01 0.186D-01-0.717D-01-0.108D+00

Coeff: 0.455D-01 0.313D+00 0.769D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=3.32D-07 MaxDP=1.27D-05 DE=-9.22D-10 OVMax= 2.66D-04

Cycle 16 Pass 1 IDiag 1:

RMSU= 1.55D-08 CP: 1.00D+00 1.08D+00 8.92D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 2.73D+00 1.78D+00 1.54D+00 1.01D+00 1.02D+00

E= -1276.01312150223 Delta-E= -0.000000000317 Rises=F Damp=F

DIIS: error= 2.20D-07 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1276.01312150223 IErMin=16 ErrMin= 2.20D-07

ErrMax= 2.20D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.66D-11 BMatP= 2.10D-10

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

Coeff-Com: -0.199D-04 0.345D-03 0.423D-03 0.139D-02 0.268D-02-0.375D-02

Coeff-Com: -0.715D-02-0.468D-02 0.132D-01 0.213D-01-0.120D-01-0.462D-01

Coeff-Com: -0.703D-01 0.708D-01 0.448D+00 0.586D+00

Coeff: -0.199D-04 0.345D-03 0.423D-03 0.139D-02 0.268D-02-0.375D-02

Coeff: -0.715D-02-0.468D-02 0.132D-01 0.213D-01-0.120D-01-0.462D-01

Coeff: -0.703D-01 0.708D-01 0.448D+00 0.586D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=6.95D-08 MaxDP=2.68D-06 DE=-3.17D-10 OVMax= 5.49D-05

Cycle 17 Pass 1 IDiag 1:

RMSU= 8.06D-09 CP: 1.00D+00 1.08D+00 8.91D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 2.73D+00 1.77D+00 1.53D+00 9.71D-01 1.18D+00

CP: 8.36D-01

E= -1276.01312150224 Delta-E= -0.000000000011 Rises=F Damp=F

DIIS: error= 1.24D-07 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=17 EnMin= -1276.01312150224 IErMin=17 ErrMin= 1.24D-07

ErrMax= 1.24D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.76D-12 BMatP= 5.66D-11

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

Coeff-Com: -0.492D-05 0.225D-04 0.635D-04 0.395D-03 0.111D-02 0.237D-02

Coeff-Com: 0.154D-02-0.998D-02-0.327D-03 0.720D-02 0.565D-02-0.571D-02

Coeff-Com: -0.448D-01-0.182D-01 0.936D-01 0.313D+00 0.654D+00

Coeff: -0.492D-05 0.225D-04 0.635D-04 0.395D-03 0.111D-02 0.237D-02

Coeff: 0.154D-02-0.998D-02-0.327D-03 0.720D-02 0.565D-02-0.571D-02

Coeff: -0.448D-01-0.182D-01 0.936D-01 0.313D+00 0.654D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=4.20D-08 MaxDP=1.61D-06 DE=-1.14D-11 OVMax= 3.35D-05

Cycle 18 Pass 1 IDiag 1:

RMSU= 2.69D-09 CP: 1.00D+00 1.08D+00 8.91D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 2.73D+00 1.78D+00 1.54D+00 9.94D-01 1.18D+00

CP: 9.25D-01 8.67D-01

E= -1276.01312150226 Delta-E= -0.000000000020 Rises=F Damp=F

DIIS: error= 2.81D-08 at cycle 18 NSaved= 18.

NSaved=18 IEnMin=18 EnMin= -1276.01312150226 IErMin=18 ErrMin= 2.81D-08

ErrMax= 2.81D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.33D-12 BMatP= 7.76D-12

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

Coeff-Com: 0.689D-06-0.469D-04-0.406D-04-0.165D-04 0.123D-03 0.199D-02

Coeff-Com: 0.216D-02-0.433D-02-0.253D-02 0.609D-04 0.502D-02 0.522D-02

Coeff-Com: -0.942D-02-0.210D-01-0.308D-01 0.621D-01 0.347D+00 0.645D+00

Coeff: 0.689D-06-0.469D-04-0.406D-04-0.165D-04 0.123D-03 0.199D-02

Coeff: 0.216D-02-0.433D-02-0.253D-02 0.609D-04 0.502D-02 0.522D-02

Coeff: -0.942D-02-0.210D-01-0.308D-01 0.621D-01 0.347D+00 0.645D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=1.13D-08 MaxDP=4.40D-07 DE=-2.00D-11 OVMax= 9.02D-06

Cycle 19 Pass 1 IDiag 1:

RMSU= 9.02D-10 CP: 1.00D+00 1.08D+00 8.91D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 2.73D+00 1.78D+00 1.53D+00 9.87D-01 1.20D+00

CP: 9.37D-01 9.86D-01 9.39D-01

E= -1276.01312150224 Delta-E= 0.000000000017 Rises=F Damp=F

DIIS: error= 1.43D-08 at cycle 19 NSaved= 19.

NSaved=19 IEnMin=18 EnMin= -1276.01312150226 IErMin=19 ErrMin= 1.43D-08

ErrMax= 1.43D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.09D-13 BMatP= 1.33D-12

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

Coeff-Com: 0.112D-05-0.285D-04-0.325D-04-0.649D-04-0.849D-04 0.701D-03

Coeff-Com: 0.835D-03-0.783D-03-0.132D-02-0.836D-03 0.175D-02 0.315D-02

Coeff-Com: 0.153D-02-0.803D-02-0.295D-01-0.104D-01 0.779D-01 0.323D+00

Coeff-Com: 0.643D+00

Coeff: 0.112D-05-0.285D-04-0.325D-04-0.649D-04-0.849D-04 0.701D-03

Coeff: 0.835D-03-0.783D-03-0.132D-02-0.836D-03 0.175D-02 0.315D-02

Coeff: 0.153D-02-0.803D-02-0.295D-01-0.104D-01 0.779D-01 0.323D+00

Coeff: 0.643D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.090 Goal= None Shift= 0.000

RMSDP=7.40D-10 MaxDP=4.45D-08 DE= 1.68D-11 OVMax= 3.97D-07

Error on total polarization charges = 0.06980

SCF Done: E(UB3LYP) = -1276.01312150 A.U. after 19 cycles

NFock= 19 Conv=0.74D-09 -V/T= 1.9659

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7705 S= 0.5102

<L.S>= 0.000000000000E+00

KE= 1.321005911081D+03 PE=-8.599574695320D+03 EE= 3.242567295781D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.71

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7705, after 0.7503

Leave Link 502 at Tue Sep 17 13:52:35 2019, MaxMem= 2415919104 cpu: 1830.5

(Enter /home/blab/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15323 LenP2D= 41234.

LDataN: DoStor=T MaxTD1= 6 Len= 172

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

GePol: Maximum number of non-zero 1st derivatives = 243

Leave Link 701 at Tue Sep 17 13:52:40 2019, MaxMem= 2415919104 cpu: 72.6

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 13:52:40 2019, MaxMem= 2415919104 cpu: 0.3

(Enter /home/blab/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

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

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

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

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

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Tue Sep 17 13:52:51 2019, MaxMem= 2415919104 cpu: 204.5

(Enter /home/blab/g09/l716.exe)

Dipole =-6.75015599D-14 7.10542736D-14 1.77635684D-15

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.002308989 -0.006217364 -0.000000000

2 7 0.005342831 0.000142847 -0.000000000

3 6 -0.009131512 0.001413193 0.000000000

4 6 0.003445477 -0.000461537 -0.000000000

5 6 -0.001096891 0.002933129 -0.000000000

6 7 0.005525139 -0.000927250 -0.000000000

7 6 -0.000853633 0.004054888 -0.000000000

8 7 -0.003858635 -0.003533283 -0.000000000

9 6 0.004581139 0.004299929 0.000000000

10 6 -0.001270770 -0.000806582 0.000000000

11 6 0.002482638 -0.001020294 -0.000000000

12 7 0.001533030 0.005407373 -0.000000000

13 6 0.001270770 0.000806582 -0.000000000

14 6 -0.002482638 0.001020294 -0.000000000

15 6 0.000853633 -0.004054888 0.000000000

16 7 0.003858635 0.003533283 0.000000000

17 6 -0.004581139 -0.004299929 -0.000000000

18 7 -0.005525139 0.000927250 -0.000000000

19 7 -0.005342831 -0.000142847 0.000000000

20 6 0.009131512 -0.001413193 0.000000000

21 6 -0.003445477 0.000461537 -0.000000000

22 6 0.001096891 -0.002933129 -0.000000000

23 6 0.002308989 0.006217364 0.000000000

24 7 -0.001533030 -0.005407373 -0.000000000

25 30 -0.000000000 0.000000000 0.000000000

26 6 -0.000529050 0.000553703 -0.000000000

27 1 0.000076878 -0.000358149 0.000000000

28 6 -0.000394228 -0.000747390 -0.000000000

29 1 0.000333245 -0.000114152 -0.000000000

30 6 0.000394228 0.000747390 -0.000000000

31 1 -0.000333245 0.000114152 -0.000000000

32 6 0.000529050 -0.000553703 -0.000000000

33 1 -0.000076878 0.000358149 0.000000000

34 1 -0.000011270 -0.000310080 -0.000000000

35 1 0.000077039 -0.000176591 0.000023574

36 1 0.000077039 -0.000176591 -0.000023574

37 1 0.000005523 0.000067493 0.000011589

38 1 0.000005523 0.000067493 -0.000011589

39 1 0.000053094 -0.000011260 -0.000000000

40 1 -0.000005523 -0.000067493 0.000011589

41 1 -0.000005523 -0.000067493 -0.000011589

42 1 -0.000053094 0.000011260 0.000000000

43 1 -0.000077039 0.000176591 0.000023574

44 1 -0.000077039 0.000176591 -0.000023574

45 1 0.000011270 0.000310080 -0.000000000

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

Cartesian Forces: Max 0.009131512 RMS 0.002237841

Leave Link 716 at Tue Sep 17 13:52:51 2019, MaxMem= 2415919104 cpu: 0.3

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

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

Internal Forces: Max 0.004907145 RMS 0.000826466

Search for a local minimum.

Step number 2 out of a maximum of 270

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

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2

DE= -5.59D-04 DEPred=-2.06D-03 R= 2.71D-01

Trust test= 2.71D-01 RLast= 1.13D-01 DXMaxT set to 3.00D-01

ITU= 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01334

Eigenvalues --- 0.01336 0.01339 0.01340 0.01610 0.01628

Eigenvalues --- 0.01642 0.01643 0.01773 0.01790 0.01812

Eigenvalues --- 0.01813 0.01890 0.01905 0.01943 0.01944

Eigenvalues --- 0.01999 0.01999 0.02046 0.02048 0.02070

Eigenvalues --- 0.02088 0.02103 0.02112 0.02113 0.02206

Eigenvalues --- 0.02314 0.02317 0.02352 0.02373 0.07190

Eigenvalues --- 0.07190 0.07195 0.07195 0.07255 0.07260

Eigenvalues --- 0.07275 0.07281 0.14494 0.14497 0.15568

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 0.16061

Eigenvalues --- 0.16498 0.18284 0.22086 0.22094 0.22702

Eigenvalues --- 0.23851 0.23853 0.23865 0.24087 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 --- 0.27300 0.32339 0.33212 0.33216 0.33275

Eigenvalues --- 0.33282 0.33282 0.33282 0.33481 0.33721

Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33843 0.34237 0.34437 0.34437

Eigenvalues --- 0.34441 0.34460 0.35534 0.35542 0.35672

Eigenvalues --- 0.35682 0.35682 0.35682 0.37183 0.39451

Eigenvalues --- 0.41670 0.41688 0.42601 0.45056 0.47944

Eigenvalues --- 0.48963 0.48996 0.49959 0.50655 0.51360

Eigenvalues --- 0.51361 0.52386 0.54016 0.54026 0.54115

Eigenvalues --- 0.56325 0.56338 0.56407 0.58388

DIIS coeff's: 1.09490 -0.09490

Cosine: 1.000 > 0.970

Length: 1.000

GDIIS step was calculated using 2 of the last 2 vectors.

Iteration 1 RMS(Cart)= 0.00316692 RMS(Int)= 0.00000542

Iteration 2 RMS(Cart)= 0.00001190 RMS(Int)= 0.00000269

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000269

ITry= 1 IFail=0 DXMaxC= 1.16D-02 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 8.74D-10 for atom 31.

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

(Linear) (Quad) (Total)

R1 2.59659 0.00252 0.00184 0.00622 0.00806 2.60465

R2 2.73877 -0.00185 -0.00229 -0.00603 -0.00832 2.73045

R3 2.53482 0.00206 -0.00034 0.00415 0.00381 2.53863

R4 2.56852 -0.00227 -0.00052 -0.00504 -0.00556 2.56296

R5 3.80591 0.00015 0.00117 0.00058 0.00174 3.80765

R6 2.77202 -0.00117 -0.00191 -0.00475 -0.00666 2.76536

R7 2.54533 0.00491 0.00116 0.01026 0.01143 2.55676

R8 2.59570 0.00158 0.00077 0.00390 0.00467 2.60037

R9 2.82183 -0.00001 0.00031 0.00010 0.00041 2.82223

R10 2.04528 0.00011 -0.00005 0.00033 0.00028 2.04556

R11 2.54497 -0.00014 0.00062 0.00026 0.00088 2.54585

R12 2.57034 -0.00166 -0.00065 -0.00398 -0.00464 2.56570

R13 2.75450 0.00145 -0.00080 0.00380 0.00301 2.75751

R14 2.59593 0.00271 0.00208 0.00643 0.00850 2.60443

R15 3.80504 0.00014 0.00108 -0.00102 0.00006 3.80509

R16 2.76430 0.00043 -0.00264 0.00056 -0.00208 2.76221

R17 2.52456 -0.00267 -0.00081 -0.00528 -0.00608 2.51848

R18 2.59258 -0.00112 0.00048 -0.00210 -0.00162 2.59096

R19 2.82124 -0.00050 0.00025 -0.00153 -0.00128 2.81996

R20 2.04479 0.00027 -0.00010 0.00078 0.00068 2.04547

R21 2.52456 -0.00267 -0.00081 -0.00528 -0.00608 2.51848

R22 2.59258 -0.00112 0.00048 -0.00210 -0.00162 2.59096

R23 2.76430 0.00043 -0.00264 0.00056 -0.00208 2.76221

R24 2.82124 -0.00050 0.00025 -0.00153 -0.00128 2.81996

R25 2.75450 0.00145 -0.00080 0.00380 0.00301 2.75751

R26 2.04479 0.00027 -0.00010 0.00078 0.00068 2.04547

R27 2.57034 -0.00166 -0.00065 -0.00398 -0.00464 2.56570

R28 2.54497 -0.00014 0.00062 0.00026 0.00088 2.54585

R29 2.59593 0.00271 0.00208 0.00643 0.00850 2.60443

R30 3.80504 0.00014 0.00108 -0.00102 0.00006 3.80509

R31 2.54533 0.00491 0.00116 0.01026 0.01143 2.55676

R32 2.56852 -0.00227 -0.00052 -0.00504 -0.00556 2.56296

R33 2.59659 0.00252 0.00184 0.00622 0.00806 2.60465

R34 3.80591 0.00015 0.00117 0.00058 0.00174 3.80765

R35 2.77202 -0.00117 -0.00191 -0.00475 -0.00666 2.76536

R36 2.59570 0.00158 0.00077 0.00390 0.00467 2.60037

R37 2.82183 -0.00001 0.00031 0.00010 0.00041 2.82223

R38 2.73877 -0.00185 -0.00229 -0.00603 -0.00832 2.73045

R39 2.04528 0.00011 -0.00005 0.00033 0.00028 2.04556

R40 2.53482 0.00206 -0.00034 0.00415 0.00381 2.53863

R41 2.06370 0.00020 -0.00022 0.00055 0.00033 2.06403

R42 2.06990 0.00010 -0.00077 0.00001 -0.00076 2.06914

R43 2.06990 0.00010 -0.00077 0.00001 -0.00076 2.06914

R44 2.06874 0.00005 -0.00088 -0.00020 -0.00108 2.06767

R45 2.06874 0.00005 -0.00088 -0.00020 -0.00108 2.06767

R46 2.06348 0.00004 -0.00024 0.00003 -0.00020 2.06327

R47 2.06874 0.00005 -0.00088 -0.00020 -0.00108 2.06767

R48 2.06874 0.00005 -0.00088 -0.00020 -0.00108 2.06767

R49 2.06348 0.00004 -0.00024 0.00003 -0.00020 2.06327

R50 2.06990 0.00010 -0.00077 0.00001 -0.00076 2.06914

R51 2.06990 0.00010 -0.00077 0.00001 -0.00076 2.06914

R52 2.06370 0.00020 -0.00022 0.00055 0.00033 2.06403

A1 1.87987 0.00017 -0.00109 0.00060 -0.00050 1.87937

A2 2.21750 -0.00160 0.00049 -0.00677 -0.00628 2.21122

A3 2.18582 0.00144 0.00060 0.00617 0.00678 2.19260

A4 1.91611 -0.00089 0.00092 -0.00338 -0.00246 1.91365

A5 2.18484 -0.00016 -0.00052 -0.00070 -0.00122 2.18363

A6 2.18223 0.00105 -0.00040 0.00408 0.00368 2.18591

A7 1.88667 0.00141 -0.00093 0.00457 0.00364 1.89031

A8 2.23293 -0.00081 0.00128 -0.00220 -0.00092 2.23201

A9 2.16359 -0.00059 -0.00035 -0.00238 -0.00272 2.16086

A10 1.85950 -0.00053 0.00080 -0.00207 -0.00127 1.85824

A11 2.16866 0.00075 -0.00086 0.00299 0.00212 2.17078

A12 2.25502 -0.00023 0.00006 -0.00092 -0.00086 2.25416

A13 1.88262 -0.00016 0.00030 0.00028 0.00058 1.88320

A14 2.17594 0.00043 -0.00022 0.00227 0.00205 2.17799

A15 2.22462 -0.00028 -0.00008 -0.00255 -0.00263 2.22199

A16 2.16922 -0.00065 -0.00169 -0.00272 -0.00441 2.16482

A17 2.22355 -0.00017 0.00106 -0.00033 0.00073 2.22428

A18 2.18076 -0.00136 0.00012 -0.00515 -0.00502 2.17573

A19 1.87888 0.00153 -0.00119 0.00548 0.00429 1.88318

A20 1.91474 -0.00114 0.00079 -0.00345 -0.00266 1.91208

A21 2.18971 0.00117 -0.00006 0.00431 0.00426 2.19397

A22 2.17873 -0.00002 -0.00074 -0.00086 -0.00160 2.17713

A23 1.88913 -0.00027 -0.00070 -0.00111 -0.00182 1.88732

A24 2.22749 -0.00088 0.00076 -0.00426 -0.00350 2.22399

A25 2.16657 0.00116 -0.00007 0.00537 0.00531 2.17188

A26 1.85337 0.00080 0.00022 0.00378 0.00400 1.85737

A27 2.17633 0.00024 -0.00014 0.00092 0.00078 2.17712

A28 2.25348 -0.00105 -0.00008 -0.00470 -0.00478 2.24870

A29 1.88865 -0.00091 0.00087 -0.00470 -0.00382 1.88483

A30 2.17234 0.00069 -0.00056 0.00391 0.00334 2.17568

A31 2.22220 0.00022 -0.00031 0.00079 0.00048 2.22268

A32 2.18495 0.00209 -0.00019 0.00945 0.00926 2.19421

A33 1.85337 0.00080 0.00022 0.00378 0.00400 1.85737

A34 2.25348 -0.00105 -0.00008 -0.00470 -0.00478 2.24870

A35 2.17633 0.00024 -0.00014 0.00092 0.00078 2.17712

A36 1.88865 -0.00091 0.00087 -0.00470 -0.00382 1.88483

A37 2.22220 0.00022 -0.00031 0.00079 0.00048 2.22268

A38 2.17234 0.00069 -0.00056 0.00391 0.00334 2.17568

A39 1.87888 0.00153 -0.00119 0.00548 0.00429 1.88318

A40 2.18076 -0.00136 0.00012 -0.00515 -0.00502 2.17573

A41 2.22355 -0.00017 0.00106 -0.00033 0.00073 2.22428

A42 1.91474 -0.00114 0.00079 -0.00345 -0.00266 1.91208

A43 2.18971 0.00117 -0.00006 0.00431 0.00426 2.19397

A44 2.17873 -0.00002 -0.00074 -0.00086 -0.00160 2.17713

A45 2.16657 0.00116 -0.00007 0.00537 0.00531 2.17188

A46 2.22749 -0.00088 0.00076 -0.00426 -0.00350 2.22399

A47 1.88913 -0.00027 -0.00070 -0.00111 -0.00182 1.88732

A48 2.16922 -0.00065 -0.00169 -0.00272 -0.00441 2.16482

A49 1.91611 -0.00089 0.00092 -0.00338 -0.00246 1.91365

A50 2.18223 0.00105 -0.00040 0.00408 0.00368 2.18591

A51 2.18484 -0.00016 -0.00052 -0.00070 -0.00122 2.18363

A52 2.23293 -0.00081 0.00128 -0.00220 -0.00092 2.23201

A53 2.16359 -0.00059 -0.00035 -0.00238 -0.00272 2.16086

A54 1.88667 0.00141 -0.00093 0.00457 0.00364 1.89031

A55 1.85950 -0.00053 0.00080 -0.00207 -0.00127 1.85824

A56 2.16866 0.00075 -0.00086 0.00299 0.00212 2.17078

A57 2.25502 -0.00023 0.00006 -0.00092 -0.00086 2.25416

A58 1.88262 -0.00016 0.00030 0.00028 0.00058 1.88320

A59 2.22462 -0.00028 -0.00008 -0.00255 -0.00263 2.22199

A60 2.17594 0.00043 -0.00022 0.00227 0.00205 2.17799

A61 1.87987 0.00017 -0.00109 0.00060 -0.00050 1.87937

A62 2.21750 -0.00160 0.00049 -0.00677 -0.00628 2.21122

A63 2.18582 0.00144 0.00060 0.00617 0.00678 2.19260

A64 2.18495 0.00209 -0.00019 0.00945 0.00926 2.19421

A65 1.56873 -0.00058 -0.00020 -0.00314 -0.00334 1.56539

A66 1.57286 0.00058 0.00020 0.00314 0.00334 1.57620

A67 1.57286 0.00058 0.00020 0.00314 0.00334 1.57620

A68 1.56873 -0.00058 -0.00020 -0.00314 -0.00334 1.56539

A69 1.94230 0.00027 0.00066 0.00219 0.00284 1.94514

A70 1.94489 0.00014 0.00079 0.00124 0.00203 1.94692

A71 1.94489 0.00014 0.00079 0.00124 0.00203 1.94692

A72 1.88533 -0.00021 -0.00055 -0.00155 -0.00210 1.88322

A73 1.88533 -0.00021 -0.00055 -0.00155 -0.00210 1.88322

A74 1.85755 -0.00018 -0.00128 -0.00191 -0.00319 1.85436

A75 1.94282 -0.00001 0.00059 0.00009 0.00069 1.94351

A76 1.94282 -0.00001 0.00059 0.00009 0.00069 1.94351

A77 1.94309 0.00007 0.00073 0.00093 0.00165 1.94474

A78 1.85944 -0.00004 -0.00110 -0.00107 -0.00216 1.85727

A79 1.88615 -0.00001 -0.00047 -0.00007 -0.00055 1.88560

A80 1.88615 -0.00001 -0.00047 -0.00007 -0.00055 1.88560

A81 1.94282 -0.00001 0.00059 0.00009 0.00069 1.94351

A82 1.94282 -0.00001 0.00059 0.00009 0.00069 1.94351

A83 1.94309 0.00007 0.00073 0.00093 0.00165 1.94474

A84 1.85944 -0.00004 -0.00110 -0.00107 -0.00216 1.85727

A85 1.88615 -0.00001 -0.00047 -0.00007 -0.00055 1.88560

A86 1.88615 -0.00001 -0.00047 -0.00007 -0.00055 1.88560

A87 1.94489 0.00014 0.00079 0.00124 0.00203 1.94692

A88 1.94489 0.00014 0.00079 0.00124 0.00203 1.94692

A89 1.94230 0.00027 0.00066 0.00219 0.00284 1.94514

A90 1.85755 -0.00018 -0.00128 -0.00191 -0.00319 1.85436

A91 1.88533 -0.00021 -0.00055 -0.00155 -0.00210 1.88322

A92 1.88533 -0.00021 -0.00055 -0.00155 -0.00210 1.88322

A93 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

A94 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

A95 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

A96 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D2 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D3 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D4 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D6 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D7 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D10 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D11 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D12 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D13 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D14 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D15 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D16 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D17 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D18 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D19 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D20 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D21 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D22 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D23 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D24 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D25 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D26 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D27 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D28 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D29 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D30 1.03604 -0.00002 -0.00028 -0.00038 -0.00067 1.03537

D31 -1.03604 0.00002 0.00028 0.00038 0.00067 -1.03537

D32 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.10556 -0.00002 -0.00028 -0.00038 -0.00067 -2.10623

D34 2.10556 0.00002 0.00028 0.00038 0.00067 2.10623

D35 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D36 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D37 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D38 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D39 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D40 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D41 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D42 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D43 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D44 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D45 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D46 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D47 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D48 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D49 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D50 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D51 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D52 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D53 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D54 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D55 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D56 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D57 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D58 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D59 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D60 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D61 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D62 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D63 1.03586 -0.00003 -0.00030 -0.00061 -0.00091 1.03495

D64 -1.03586 0.00003 0.00030 0.00061 0.00091 -1.03495

D65 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D66 -2.10573 -0.00003 -0.00030 -0.00061 -0.00091 -2.10664

D67 2.10573 0.00003 0.00030 0.00061 0.00091 2.10664

D68 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D69 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D70 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D71 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D72 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D73 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D74 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D75 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D76 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D77 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D78 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D79 -2.10573 -0.00003 -0.00030 -0.00061 -0.00091 -2.10664

D80 2.10573 0.00003 0.00030 0.00061 0.00091 2.10664

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 1.03586 -0.00003 -0.00030 -0.00061 -0.00091 1.03495

D83 -1.03586 0.00003 0.00030 0.00061 0.00091 -1.03495

D84 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D85 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D86 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D87 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D88 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D89 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D90 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D91 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D92 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D93 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D94 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D95 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D96 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D97 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D98 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D99 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D100 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D101 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D102 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D103 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D104 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D105 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D106 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D107 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D108 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D109 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D110 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D111 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D112 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D113 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D114 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D116 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D117 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D118 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D119 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D120 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D121 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D122 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D123 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D124 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D125 1.03604 -0.00002 -0.00028 -0.00038 -0.00067 1.03537

D126 -1.03604 0.00002 0.00028 0.00038 0.00067 -1.03537

D127 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D128 -2.10556 -0.00002 -0.00028 -0.00038 -0.00067 -2.10623

D129 2.10556 0.00002 0.00028 0.00038 0.00067 2.10623

D130 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D131 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D132 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D133 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D134 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D135 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D136 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

Item Value Threshold Converged?

Maximum Force 0.004907 0.000450 NO

RMS Force 0.000826 0.000300 NO

Maximum Displacement 0.011564 0.001800 NO

RMS Displacement 0.003160 0.001200 NO

Predicted change in Energy=-2.924255D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 13:52:51 2019, MaxMem= 2415919104 cpu: 1.6

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.084796 -2.192739 -0.000000

2 7 0 -0.744208 -1.872447 -0.000000

3 6 0 -0.003922 -3.008852 -0.000000

4 6 0 -0.917116 -4.152317 -0.000000

5 6 0 -2.191690 -3.633669 -0.000000

6 7 0 1.344305 -3.122143 -0.000000

7 6 0 2.189169 -2.072775 -0.000000

8 7 0 1.867145 -0.753808 -0.000000

9 6 0 3.019395 0.002348 -0.000000

10 6 0 4.161904 -0.909378 -0.000000

11 6 0 3.644502 -2.179081 -0.000000

12 7 0 -3.115854 -1.331576 -0.000000

13 6 0 -4.161904 0.909378 -0.000000

14 6 0 -3.644502 2.179081 -0.000000

15 6 0 -2.189169 2.072775 -0.000000

16 7 0 -1.867145 0.753808 -0.000000

17 6 0 -3.019395 -0.002348 -0.000000

18 7 0 -1.344305 3.122143 -0.000000

19 7 0 0.744208 1.872447 -0.000000

20 6 0 0.003922 3.008852 -0.000000

21 6 0 0.917116 4.152317 -0.000000

22 6 0 2.191690 3.633669 -0.000000

23 6 0 2.084796 2.192739 -0.000000

24 7 0 3.115854 1.331576 -0.000000

25 30 0 0.000000 -0.000000 -0.000000

26 6 0 -0.480179 -5.580434 -0.000000

27 1 0 -3.123920 -4.183825 -0.000000

28 6 0 5.591445 -0.481300 -0.000000

29 1 0 4.193532 -3.111923 -0.000000

30 6 0 -5.591445 0.481300 -0.000000

31 1 0 -4.193532 3.111923 -0.000000

32 6 0 0.480179 5.580434 -0.000000

33 1 0 3.123920 4.183825 -0.000000

34 1 0 -1.335447 -6.259770 -0.000000

35 1 0 0.134353 -5.813006 0.875878

36 1 0 0.134353 -5.813006 -0.875878

37 1 0 5.823877 0.131417 0.876209

38 1 0 5.823877 0.131417 -0.876209

39 1 0 6.265086 -1.340555 -0.000000

40 1 0 -5.823877 -0.131417 0.876209

41 1 0 -5.823877 -0.131417 -0.876209

42 1 0 -6.265086 1.340555 -0.000000

43 1 0 -0.134353 5.813006 0.875878

44 1 0 -0.134353 5.813006 -0.875878

45 1 0 1.335447 6.259770 -0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.378319 0.000000

3 C 2.235191 1.356259 0.000000

4 C 2.281102 2.286417 1.463365 0.000000

5 C 1.444890 2.279716 2.275242 1.376058 0.000000

6 N 3.552820 2.433851 1.352979 2.485012 3.572803

7 C 4.275649 2.940210 2.384510 3.738115 4.650625

8 N 4.205754 2.840866 2.930207 4.393402 4.976720

9 C 5.556184 4.204708 4.267057 5.723405 6.354214

10 C 6.377168 4.999743 4.664964 6.026035 6.913025

11 C 5.729314 4.399409 3.741592 4.970113 6.014729

12 N 1.343384 2.432539 3.535163 3.576455 2.480668

13 C 3.733296 4.406721 5.713260 6.012437 4.951870

14 C 4.641712 4.982629 6.337860 6.893855 5.991555

15 C 4.266790 4.201510 5.531567 6.353730 5.706444

16 N 2.954574 2.856257 4.198715 4.997261 4.399464

17 C 2.381446 2.945123 4.258186 4.652077 3.724458

18 N 5.366218 5.030512 6.275805 7.286993 6.808749

19 N 4.952676 4.029841 4.938297 6.249623 6.239937

20 C 5.605291 4.938297 6.017709 7.220156 6.995984

21 C 7.019346 6.249623 7.220156 8.504785 8.383690

22 C 7.227404 6.239937 6.995984 8.383690 8.486944

23 C 6.051274 4.952676 5.605291 7.019346 7.227404

24 N 6.282321 5.016557 5.345307 6.807197 7.267990

25 Zn 3.025637 2.014921 3.008854 4.252392 4.243472

26 C 3.748503 3.717375 2.615311 1.493462 2.592134

27 H 2.245930 3.317453 3.333909 2.207029 1.082462

28 C 7.864712 6.486585 6.139759 7.472465 8.397298

29 H 6.345259 5.090931 4.198719 5.215472 6.406503

30 C 4.409883 5.388491 6.587987 6.581775 5.337725

31 H 5.708432 6.061500 7.417326 7.968945 7.036361

32 C 8.185433 7.552785 8.602917 9.832542 9.593674

33 H 8.233546 7.186157 7.843340 9.263975 9.453514

34 H 4.135489 4.426981 3.513037 2.148571 2.762165

35 H 4.335680 4.131227 2.941014 2.151891 3.305623

36 H 4.335680 4.131227 2.941014 2.151891 3.305623

37 H 8.289545 6.922641 6.677745 8.034869 8.899041

38 H 8.289545 6.922641 6.677745 8.034869 8.899041

39 H 8.393257 7.029446 6.487193 7.712979 8.762159

40 H 4.358614 5.440769 6.551279 6.404037 5.121162

41 H 4.358614 5.440769 6.551279 6.404037 5.121162

42 H 5.473480 6.387760 7.623616 7.666318 6.429266

43 H 8.286334 7.759206 8.866191 10.034318 9.707701

44 H 8.286334 7.759206 8.866191 10.034318 9.707701

45 H 9.118277 8.393922 9.364895 10.652962 10.503373

6 7 8 9 10

6 N 0.000000

7 C 1.347208 0.000000

8 N 2.425361 1.357709 0.000000

9 C 3.545190 2.235042 1.378206 0.000000

10 C 3.582623 2.290234 2.300025 1.461701 0.000000

11 C 2.486015 1.459210 2.278245 2.269227 1.371077

12 N 4.806158 5.356552 5.016383 6.278586 7.289993

13 C 6.824331 7.016363 6.254248 7.238353 8.520190

14 C 7.279504 7.218725 6.243404 7.010399 8.395150

15 C 6.282724 6.029546 4.944012 5.604981 7.016363

16 N 5.033529 4.944012 4.027137 4.943984 6.254248

17 C 5.364234 5.604981 4.943984 6.038793 7.238353

18 N 6.798510 6.282724 5.033529 5.364234 6.824331

19 N 5.030512 4.201510 2.856257 2.945123 4.406721

20 C 6.275805 5.531567 4.198715 4.258186 5.713260

21 C 7.286993 6.353730 4.997261 4.652077 6.012437

22 C 6.808749 5.706444 4.399464 3.724458 4.951870

23 C 5.366218 4.266790 2.954574 2.381446 3.733296

24 N 4.793120 3.528222 2.430658 1.332723 2.473074

25 Zn 3.399255 3.014773 2.013569 3.019396 4.260095

26 C 3.061362 4.407844 5.367145 6.588966 6.585415

27 H 4.592625 5.717119 6.056051 7.434001 7.987817

28 C 5.001224 3.756098 3.734256 2.617127 1.492259

29 H 2.849245 2.257720 3.312519 3.328255 2.202772

30 C 7.815973 8.189093 7.560163 8.624150 9.851994

31 H 8.338538 8.223136 7.188580 7.854666 9.272765

32 C 8.745374 7.841699 6.484311 6.128838 7.461417

33 H 7.519588 6.326041 5.095066 4.182783 5.197896

34 H 4.126230 5.473011 6.369633 7.627502 7.671217

35 H 3.077643 4.356462 5.418968 6.550494 6.405770

36 H 3.077643 4.356462 5.418968 6.550494 6.405770

37 H 5.605351 4.340197 4.148143 2.941007 2.147825

38 H 5.605351 4.340197 4.148143 2.941007 2.147825

39 H 5.233368 4.141165 4.436908 3.512534 2.146926

40 H 7.816331 8.291292 7.765755 8.887582 10.054292

41 H 7.816331 8.291292 7.765755 8.887582 10.054292

42 H 8.821480 9.117305 8.397592 9.380426 10.666973

43 H 9.098928 8.267494 6.920708 6.669110 8.025922

44 H 9.098928 8.267494 6.920708 6.669110 8.025922

45 H 9.381918 8.376165 7.033703 6.480047 7.706201

11 12 13 14 15

11 C 0.000000

12 N 6.813272 0.000000

13 C 8.395150 2.473074 0.000000

14 C 8.492535 3.550237 1.371077 0.000000

15 C 7.218725 3.528222 2.290234 1.459210 0.000000

16 N 6.243404 2.430658 2.300025 2.278245 1.357709

17 C 7.010399 1.332723 1.461701 2.269227 2.235042

18 N 7.279504 4.793120 3.582623 2.486015 1.347208

19 N 4.982629 5.016557 4.999743 4.399409 2.940210

20 C 6.337860 5.345307 4.664964 3.741592 2.384510

21 C 6.893855 6.807197 6.026035 4.970113 3.738115

22 C 5.991555 7.267990 6.913025 6.014729 4.650625

23 C 4.641712 6.282321 6.377168 5.729314 4.275649

24 N 3.550237 6.776914 7.289993 6.813272 5.356552

25 Zn 4.246268 3.388457 4.260095 4.246268 3.014773

26 C 5.346232 4.999957 7.461417 8.379917 7.841699

27 H 7.059074 2.852260 5.197896 6.384166 6.326041

28 C 2.583224 8.748715 9.851994 9.611469 8.189093

29 H 1.082417 7.523082 9.272765 9.456717 8.223136

30 C 9.611469 3.068399 1.492259 2.583224 3.756098

31 H 9.456717 4.572315 2.202772 1.082417 2.257720

32 C 8.379917 7.791491 6.585415 5.346232 4.407844

33 H 6.384166 8.327930 7.987817 7.059074 5.717119

34 H 6.438316 5.239938 7.706201 8.749054 8.376165

35 H 5.127740 5.604839 8.025922 8.883713 8.267494

36 H 5.127740 5.604839 8.025922 8.883713 8.267494

37 H 3.294817 9.100928 10.054292 9.726812 8.291292

38 H 3.294817 9.100928 10.054292 9.726812 8.291292

39 H 2.751470 9.380944 10.666973 10.516072 9.117305

40 H 9.726812 3.088934 2.147825 3.294817 4.340197

41 H 9.726812 3.088934 2.147825 3.294817 4.340197

42 H 10.516072 4.130126 2.146926 2.751470 4.141165

43 H 8.883713 7.791120 6.405770 5.127740 4.356462

44 H 8.883713 7.791120 6.405770 5.127740 4.356462

45 H 8.749054 8.800149 7.671217 6.438316 5.473011

16 17 18 19 20

16 N 0.000000

17 C 1.378206 0.000000

18 N 2.425361 3.545190 0.000000

19 N 2.840866 4.204708 2.433851 0.000000

20 C 2.930207 4.267057 1.352979 1.356259 0.000000

21 C 4.393402 5.723405 2.485012 2.286417 1.463365

22 C 4.976720 6.354214 3.572803 2.279716 2.275242

23 C 4.205754 5.556184 3.552820 1.378319 2.235191

24 N 5.016383 6.278586 4.806158 2.432539 3.535163

25 Zn 2.013569 3.019396 3.399255 2.014921 3.008854

26 C 6.484311 6.128838 8.745374 7.552785 8.602917

27 H 5.095066 4.182783 7.519588 7.186157 7.843340

28 C 7.560163 8.624150 7.815973 5.388491 6.587987

29 H 7.188580 7.854666 8.338538 6.061500 7.417326

30 C 3.734256 2.617127 5.001224 6.486585 6.139759

31 H 3.312519 3.328255 2.849245 5.090931 4.198719

32 C 5.367145 6.588966 3.061362 3.717375 2.615311

33 H 6.056051 7.434001 4.592625 3.317453 3.333909

34 H 7.033703 6.480047 9.381918 8.393922 9.364895

35 H 6.920708 6.669110 9.098928 7.759206 8.866191

36 H 6.920708 6.669110 9.098928 7.759206 8.866191

37 H 7.765755 8.887582 7.816331 5.440769 6.551279

38 H 7.765755 8.887582 7.816331 5.440769 6.551279

39 H 8.397592 9.380426 8.821480 6.387760 7.623616

40 H 4.148143 2.941007 5.605351 6.922641 6.677745

41 H 4.148143 2.941007 5.605351 6.922641 6.677745

42 H 4.436908 3.512534 5.233368 7.029446 6.487193

43 H 5.418968 6.550494 3.077643 4.131227 2.941014

44 H 5.418968 6.550494 3.077643 4.131227 2.941014

45 H 6.369633 7.627502 4.126230 4.426981 3.513037

21 22 23 24 25

21 C 0.000000

22 C 1.376058 0.000000

23 C 2.281102 1.444890 0.000000

24 N 3.576455 2.480668 1.343384 0.000000

25 Zn 4.252392 4.243472 3.025637 3.388457 0.000000

26 C 9.832542 9.593674 8.185433 7.791491 5.601054

27 H 9.263975 9.453514 8.233546 8.327930 5.221424

28 C 6.581775 5.337725 4.409883 3.068399 5.612121

29 H 7.968945 7.036361 5.708432 4.572315 5.222047

30 C 7.472465 8.397298 7.864712 8.748715 5.612121

31 H 5.215472 6.406503 6.345259 7.523082 5.222047

32 C 1.493462 2.592134 3.748503 4.999957 5.601054

33 H 2.207029 1.082462 2.245930 2.852260 5.221424

34 H 10.652962 10.503373 9.118277 8.800149 6.400636

35 H 10.034318 9.707701 8.286334 7.791120 5.880157

36 H 10.034318 9.707701 8.286334 7.791120 5.880157

37 H 6.404037 5.121162 4.358614 3.088934 5.890888

38 H 6.404037 5.121162 4.358614 3.088934 5.890888

39 H 7.666318 6.429266 5.473480 4.130126 6.406902

40 H 8.034869 8.899041 8.289545 9.100928 5.890888

41 H 8.034869 8.899041 8.289545 9.100928 5.890888

42 H 7.712979 8.762159 8.393257 9.380944 6.406902

43 H 2.151891 3.305623 4.335680 5.604839 5.880157

44 H 2.151891 3.305623 4.335680 5.604839 5.880157

45 H 2.148571 2.762165 4.135489 5.239938 6.400636

26 27 28 29 30

26 C 0.000000

27 H 2.989964 0.000000

28 C 7.928794 9.469227 0.000000

29 H 5.285558 7.395545 2.978982 0.000000

30 C 7.929039 5.277506 11.224242 10.423868 0.000000

31 H 9.452304 7.373737 10.423868 10.444094 2.978982

32 C 11.202109 10.408183 7.929039 9.452304 7.928794

33 H 10.408183 10.442847 5.277506 7.373737 9.469227

34 H 1.092237 2.740107 9.020673 6.362276 7.972173

35 H 1.094943 3.746696 7.679459 4.953781 8.553959

36 H 1.094943 3.746696 7.679459 4.953781 8.553959

37 H 8.551848 9.972569 1.094162 3.734303 11.454246

38 H 8.551848 9.972569 1.094162 3.734303 11.454246

39 H 7.967131 9.810078 1.091838 2.725634 11.995686

40 H 7.682099 4.947679 11.454246 10.488072 1.094162

41 H 7.682099 4.947679 11.454246 10.488072 1.094162

42 H 9.020267 6.354974 11.995686 11.366937 1.091838

43 H 11.432288 10.470974 8.553959 9.957515 7.679459

44 H 11.432288 10.470974 8.553959 9.957515 7.679459

45 H 11.978603 11.355819 7.972173 9.797820 9.020673

31 32 33 34 35

31 H 0.000000

32 C 5.285558 0.000000

33 H 7.395545 2.989964 0.000000

34 H 9.797820 11.978603 11.355819 0.000000

35 H 9.957515 11.432288 10.470974 1.768353 0.000000

36 H 9.957515 11.432288 10.470974 1.768353 1.751755

37 H 10.488072 7.682099 4.947679 9.636957 8.228417

38 H 10.488072 7.682099 4.947679 9.636957 8.412886

39 H 11.366937 9.020267 6.354974 9.053551 7.639102

40 H 3.734303 8.551848 9.972569 7.646598 8.232920

41 H 3.734303 8.551848 9.972569 7.646598 8.417290

42 H 2.725634 7.967131 9.810078 9.059044 9.638123

43 H 4.953781 1.094943 3.746696 12.163951 11.629117

44 H 4.953781 1.094943 3.746696 12.163951 11.760315

45 H 6.362276 1.092237 2.740107 12.801272 12.163951

36 37 38 39 40

36 H 0.000000

37 H 8.412886 0.000000

38 H 8.228417 1.752418 0.000000

39 H 7.639102 1.768928 1.768928 0.000000

40 H 8.417290 11.650720 11.781776 12.180837 0.000000

41 H 8.232920 11.781776 11.650720 12.180837 1.752418

42 H 9.638123 12.180837 12.180837 12.813804 1.768928

43 H 11.760315 8.232920 8.417290 9.638123 8.228417

44 H 11.629117 8.417290 8.232920 9.638123 8.412886

45 H 12.163951 7.646598 7.646598 9.059044 9.636957

41 42 43 44 45

41 H 0.000000

42 H 1.768928 0.000000

43 H 8.412886 7.639102 0.000000

44 H 8.228417 7.639102 1.751755 0.000000

45 H 9.636957 9.053551 1.768353 1.768353 0.000000

Stoichiometry C20H16N8Zn(1-,2)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=3 Diff= 2.21D-03

Largest Abelian subgroup C2H NOp 4

Largest concise Abelian subgroup C2H NOp 4

Standard orientation:

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.813760 1.112311 0.000000

2 7 0 -2.014891 -0.010886 0.000000

3 6 0 -2.791522 -1.122770 0.000000

4 6 0 -4.193704 -0.704054 0.000000

5 6 0 -4.189925 0.671999 0.000000

6 7 0 -2.391847 -2.415368 0.000000

7 6 0 -1.102500 -2.805949 0.000000

8 7 0 0.000000 -2.013569 0.000000

9 6 0 1.132531 -2.798951 0.000000

10 6 0 0.714818 -4.199696 0.000000

11 6 0 -0.656252 -4.195250 0.000000

12 7 0 -2.401210 2.390780 0.000000

13 6 0 -0.714818 4.199696 0.000000

14 6 0 0.656252 4.195250 0.000000

15 6 0 1.102500 2.805949 0.000000

16 7 0 0.000000 2.013569 0.000000

17 6 0 -1.132531 2.798951 0.000000

18 7 0 2.391847 2.415368 0.000000

19 7 0 2.014891 0.010886 0.000000

20 6 0 2.791522 1.122770 0.000000

21 6 0 4.193704 0.704054 0.000000

22 6 0 4.189925 -0.671999 0.000000

23 6 0 2.813760 -1.112311 0.000000

24 7 0 2.401210 -2.390780 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -5.354396 -1.643853 0.000000

27 1 0 -5.049068 1.330480 0.000000

28 6 0 1.646935 -5.365026 0.000000

29 1 0 -1.315721 -5.053578 0.000000

30 6 0 -1.646935 5.365026 0.000000

31 1 0 1.315721 5.053578 0.000000

32 6 0 5.354396 1.643853 0.000000

33 1 0 5.049068 -1.330480 0.000000

34 1 0 -6.304514 -1.105097 0.000000

35 1 0 -5.339998 -2.300764 0.875878

36 1 0 -5.339998 -2.300764 -0.875878

37 1 0 2.302111 -5.351178 0.876209

38 1 0 2.302111 -5.351178 -0.876209

39 1 0 1.102352 -6.311356 0.000000

40 1 0 -2.302111 5.351178 0.876209

41 1 0 -2.302111 5.351178 -0.876209

42 1 0 -1.102352 6.311356 0.000000

43 1 0 5.339998 2.300764 0.875878

44 1 0 5.339998 2.300764 -0.875878

45 1 0 6.304514 1.105097 0.000000

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

Rotational constants (GHZ): 0.1824558 0.1817611 0.0912574

Leave Link 202 at Tue Sep 17 13:52:51 2019, MaxMem= 2415919104 cpu: 0.2

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 229 symmetry adapted cartesian basis functions of AG symmetry.

There are 82 symmetry adapted cartesian basis functions of BG symmetry.

There are 78 symmetry adapted cartesian basis functions of AU symmetry.

There are 218 symmetry adapted cartesian basis functions of BU symmetry.

There are 212 symmetry adapted basis functions of AG symmetry.

There are 82 symmetry adapted basis functions of BG symmetry.

There are 78 symmetry adapted basis functions of AU symmetry.

There are 204 symmetry adapted basis functions of BU symmetry.

576 basis functions, 1015 primitive gaussians, 607 cartesian basis functions

103 alpha electrons 102 beta electrons

nuclear repulsion energy 2759.4506561441 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= 45 NActive= 45 NUniq= 21 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1141555888 Hartrees.

Nuclear repulsion after empirical dispersion term = 2759.3365005553 Hartrees.

No density basis found on file 724.

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

Polarizable Continuum Model (PCM)

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

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

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 = 45

GePol: Total number of spheres = 45

GePol: Number of exposed spheres = 45 (100.00%)

GePol: Number of points = 3490

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.23D-07

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 132

GePol: Fraction of low-weight points (<1% of avg) = 3.78%

GePol: Cavity surface area = 382.151 Ang\*\*2

GePol: Cavity volume = 379.243 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0106792216 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2759.3258213338 Hartrees.

Leave Link 301 at Tue Sep 17 13:52:51 2019, MaxMem= 2415919104 cpu: 2.0

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15319 LenP2D= 41220.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.79D-04 NBF= 212 82 78 204

NBsUse= 576 1.00D-06 EigRej= -1.00D+00 NBFU= 212 82 78 204

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= 594 594 594 594 594 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Tue Sep 17 13:52:52 2019, MaxMem= 2415919104 cpu: 12.5

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 13:52:52 2019, MaxMem= 2415919104 cpu: 1.3

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

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

B after Tr= 0.000000 0.000000 -0.000000

Rot= 1.000000 0.000000 -0.000000 -0.000795 Ang= -0.09 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-BG.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7705 S= 0.5102

Leave Link 401 at Tue Sep 17 13:52:53 2019, MaxMem= 2415919104 cpu: 20.2

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1141655 IEndB= 1141655 NGot= 2415919104 MDV= 2415163146

LenX= 2415163146 LenY= 2414794090

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= 670000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 36540300.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.55D-15 for 3486.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.79D-15 for 1185 268.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.77D-15 for 3486.

Iteration 1 A^-1\*A deviation from orthogonality is 4.25D-14 for 3270 3131.

E= -1276.01327155717

DIIS: error= 4.11D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1276.01327155717 IErMin= 1 ErrMin= 4.11D-04

ErrMax= 4.11D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.97D-04 BMatP= 5.97D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 4.11D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.288 Goal= None Shift= 0.000

Gap= 0.342 Goal= None Shift= 0.000

RMSDP=4.24D-05 MaxDP=1.03D-03 OVMax= 1.94D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.24D-05 CP: 1.00D+00

E= -1276.01348335247 Delta-E= -0.000211795302 Rises=F Damp=F

DIIS: error= 3.61D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1276.01348335247 IErMin= 2 ErrMin= 3.61D-04

ErrMax= 3.61D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.12D-04 BMatP= 5.97D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.61D-03

Coeff-Com: 0.184D+00 0.816D+00

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

Coeff: 0.184D+00 0.816D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=1.92D-05 MaxDP=1.10D-03 DE=-2.12D-04 OVMax= 7.70D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.87D-05 CP: 1.00D+00 1.10D+00

E= -1276.01348306237 Delta-E= 0.000000290101 Rises=F Damp=F

DIIS: error= 5.48D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1276.01348335247 IErMin= 2 ErrMin= 3.61D-04

ErrMax= 5.48D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.55D-04 BMatP= 1.12D-04

IDIUse=3 WtCom= 2.99D-01 WtEn= 7.01D-01

Coeff-Com: -0.126D-01 0.548D+00 0.465D+00

Coeff-En: 0.000D+00 0.502D+00 0.498D+00

Coeff: -0.377D-02 0.516D+00 0.488D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=1.72D-05 MaxDP=6.77D-04 DE= 2.90D-07 OVMax= 9.83D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.35D-05 CP: 1.00D+00 1.30D+00 6.56D-01

E= -1276.01352530757 Delta-E= -0.000042245201 Rises=F Damp=F

DIIS: error= 1.84D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1276.01352530757 IErMin= 4 ErrMin= 1.84D-04

ErrMax= 1.84D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.53D-05 BMatP= 1.12D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.84D-03

Coeff-Com: -0.110D-01 0.134D+00 0.277D+00 0.601D+00

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

Coeff: -0.110D-01 0.134D+00 0.276D+00 0.601D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=9.62D-06 MaxDP=3.41D-04 DE=-4.22D-05 OVMax= 7.23D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.31D-06 CP: 1.00D+00 1.41D+00 9.78D-01 1.36D+00

E= -1276.01353602911 Delta-E= -0.000010721541 Rises=F Damp=F

DIIS: error= 1.59D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1276.01353602911 IErMin= 5 ErrMin= 1.59D-04

ErrMax= 1.59D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.68D-06 BMatP= 1.53D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.59D-03

Coeff-Com: -0.278D-02-0.263D-01 0.121D+00 0.380D+00 0.528D+00

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

Coeff: -0.277D-02-0.262D-01 0.121D+00 0.380D+00 0.528D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=8.23D-06 MaxDP=3.30D-04 DE=-1.07D-05 OVMax= 6.57D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.28D-06 CP: 1.00D+00 1.51D+00 1.16D+00 1.80D+00 1.26D+00

E= -1276.01354291586 Delta-E= -0.000006886752 Rises=F Damp=F

DIIS: error= 1.47D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1276.01354291586 IErMin= 6 ErrMin= 1.47D-04

ErrMax= 1.47D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.05D-06 BMatP= 3.68D-06

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.47D-03

Coeff-Com: 0.950D-02-0.145D+00-0.113D+00-0.367D+00-0.179D+00 0.179D+01

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

Coeff: 0.949D-02-0.145D+00-0.113D+00-0.366D+00-0.178D+00 0.179D+01

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=2.53D-05 MaxDP=9.97D-04 DE=-6.89D-06 OVMax= 2.03D-02

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.95D-06 CP: 1.00D+00 1.82D+00 1.76D+00 3.00D+00 2.73D+00

CP: 2.81D+00

E= -1276.01355980223 Delta-E= -0.000016886365 Rises=F Damp=F

DIIS: error= 1.04D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1276.01355980223 IErMin= 7 ErrMin= 1.04D-04

ErrMax= 1.04D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.45D-06 BMatP= 2.05D-06

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.04D-03

Coeff-Com: 0.102D-01-0.108D+00-0.162D+00-0.635D+00-0.752D+00 0.141D+01

Coeff-Com: 0.123D+01

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: 0.102D-01-0.108D+00-0.162D+00-0.635D+00-0.751D+00 0.141D+01

Coeff: 0.123D+01

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=3.49D-05 MaxDP=1.37D-03 DE=-1.69D-05 OVMax= 2.80D-02

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.28D-05 CP: 1.00D+00 2.25D+00 2.58D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00

E= -1276.01357460515 Delta-E= -0.000014802920 Rises=F Damp=F

DIIS: error= 5.10D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1276.01357460515 IErMin= 8 ErrMin= 5.10D-05

ErrMax= 5.10D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.95D-07 BMatP= 1.45D-06

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

Coeff-Com: -0.295D-02 0.740D-01 0.860D-01 0.828D-01-0.197D+00-0.758D+00

Coeff-Com: 0.750D+00 0.965D+00

Coeff: -0.295D-02 0.740D-01 0.860D-01 0.828D-01-0.197D+00-0.758D+00

Coeff: 0.750D+00 0.965D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=1.43D-05 MaxDP=5.68D-04 DE=-1.48D-05 OVMax= 1.15D-02

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.28D-06 CP: 1.00D+00 2.43D+00 2.91D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.45D+00

E= -1276.01357801244 Delta-E= -0.000003407297 Rises=F Damp=F

DIIS: error= 3.18D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1276.01357801244 IErMin= 9 ErrMin= 3.18D-05

ErrMax= 3.18D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.85D-07 BMatP= 6.95D-07

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

Coeff-Com: -0.397D-02 0.585D-01 0.796D-01 0.158D+00 0.343D-01-0.770D+00

Coeff-Com: 0.114D+00 0.419D+00 0.911D+00

Coeff: -0.397D-02 0.585D-01 0.796D-01 0.158D+00 0.343D-01-0.770D+00

Coeff: 0.114D+00 0.419D+00 0.911D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=1.46D-05 MaxDP=5.67D-04 DE=-3.41D-06 OVMax= 1.17D-02

Cycle 10 Pass 1 IDiag 1:

RMSU= 4.85D-06 CP: 1.00D+00 2.60D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.92D+00 1.93D+00

E= -1276.01357964964 Delta-E= -0.000001637193 Rises=F Damp=F

DIIS: error= 1.42D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1276.01357964964 IErMin=10 ErrMin= 1.42D-05

ErrMax= 1.42D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.34D-07 BMatP= 2.85D-07

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

Coeff-Com: -0.633D-03-0.122D-01 0.219D-01 0.116D+00 0.247D+00 0.380D-01

Coeff-Com: -0.502D+00-0.474D+00 0.538D+00 0.103D+01

Coeff: -0.633D-03-0.122D-01 0.219D-01 0.116D+00 0.247D+00 0.380D-01

Coeff: -0.502D+00-0.474D+00 0.538D+00 0.103D+01

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=1.86D-06 MaxDP=6.07D-05 DE=-1.64D-06 OVMax= 1.21D-03

Cycle 11 Pass 1 IDiag 1:

RMSU= 8.86D-07 CP: 1.00D+00 2.58D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.86D+00 2.08D+00 8.65D-01

E= -1276.01357966840 Delta-E= -0.000000018763 Rises=F Damp=F

DIIS: error= 1.52D-05 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1276.01357966840 IErMin=10 ErrMin= 1.42D-05

ErrMax= 1.52D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.16D-07 BMatP= 1.34D-07

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

Coeff-Com: 0.102D-02-0.251D-01-0.220D-01-0.156D-01 0.567D-01 0.242D+00

Coeff-Com: -0.257D+00-0.209D+00-0.146D+00 0.692D+00 0.683D+00

Coeff: 0.102D-02-0.251D-01-0.220D-01-0.156D-01 0.567D-01 0.242D+00

Coeff: -0.257D+00-0.209D+00-0.146D+00 0.692D+00 0.683D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=5.59D-06 MaxDP=2.15D-04 DE=-1.88D-08 OVMax= 4.47D-03

Cycle 12 Pass 1 IDiag 1:

RMSU= 2.03D-07 CP: 1.00D+00 2.65D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.04D+00 2.41D+00 1.36D+00

CP: 9.62D-01

E= -1276.01357990373 Delta-E= -0.000000235330 Rises=F Damp=F

DIIS: error= 2.64D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1276.01357990373 IErMin=12 ErrMin= 2.64D-06

ErrMax= 2.64D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.11D-08 BMatP= 1.16D-07

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

Coeff-Com: 0.788D-03-0.126D-01-0.171D-01-0.314D-01-0.188D-01 0.146D+00

Coeff-Com: -0.584D-01-0.465D-02-0.245D+00 0.243D+00 0.372D+00 0.626D+00

Coeff: 0.788D-03-0.126D-01-0.171D-01-0.314D-01-0.188D-01 0.146D+00

Coeff: -0.584D-01-0.465D-02-0.245D+00 0.243D+00 0.372D+00 0.626D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=1.10D-06 MaxDP=4.26D-05 DE=-2.35D-07 OVMax= 8.81D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 9.32D-08 CP: 1.00D+00 2.67D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.08D+00 2.48D+00 1.46D+00

CP: 9.86D-01 1.05D+00

E= -1276.01357991799 Delta-E= -0.000000014257 Rises=F Damp=F

DIIS: error= 1.10D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1276.01357991799 IErMin=13 ErrMin= 1.10D-06

ErrMax= 1.10D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.57D-09 BMatP= 1.11D-08

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

Coeff-Com: 0.104D-03 0.426D-03-0.152D-02-0.900D-02-0.222D-01 0.102D-01

Coeff-Com: 0.323D-01 0.445D-01-0.824D-01-0.507D-01-0.566D-02 0.295D+00

Coeff-Com: 0.789D+00

Coeff: 0.104D-03 0.426D-03-0.152D-02-0.900D-02-0.222D-01 0.102D-01

Coeff: 0.323D-01 0.445D-01-0.824D-01-0.507D-01-0.566D-02 0.295D+00

Coeff: 0.789D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=3.48D-07 MaxDP=1.27D-05 DE=-1.43D-08 OVMax= 2.75D-04

Cycle 14 Pass 1 IDiag 1:

RMSU= 4.23D-08 CP: 1.00D+00 2.67D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.09D+00 2.50D+00 1.49D+00

CP: 1.02D+00 1.22D+00 1.06D+00

E= -1276.01357992030 Delta-E= -0.000000002314 Rises=F Damp=F

DIIS: error= 8.87D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1276.01357992030 IErMin=14 ErrMin= 8.87D-07

ErrMax= 8.87D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.39D-10 BMatP= 1.57D-09

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

Coeff-Com: -0.115D-03 0.322D-02 0.325D-02 0.136D-02-0.102D-01-0.281D-01

Coeff-Com: 0.338D-01 0.241D-01 0.830D-02-0.936D-01-0.957D-01 0.417D-01

Coeff-Com: 0.512D+00 0.599D+00

Coeff: -0.115D-03 0.322D-02 0.325D-02 0.136D-02-0.102D-01-0.281D-01

Coeff: 0.338D-01 0.241D-01 0.830D-02-0.936D-01-0.957D-01 0.417D-01

Coeff: 0.512D+00 0.599D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=3.52D-07 MaxDP=1.34D-05 DE=-2.31D-09 OVMax= 2.81D-04

Cycle 15 Pass 1 IDiag 1:

RMSU= 1.99D-08 CP: 1.00D+00 2.67D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.10D+00 2.53D+00 1.52D+00

CP: 1.03D+00 1.29D+00 1.23D+00 1.00D+00

E= -1276.01357992124 Delta-E= -0.000000000943 Rises=F Damp=F

DIIS: error= 3.19D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1276.01357992124 IErMin=15 ErrMin= 3.19D-07

ErrMax= 3.19D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.46D-11 BMatP= 7.39D-10

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

Coeff-Com: -0.416D-04 0.405D-03 0.110D-02 0.162D-02 0.204D-02-0.569D-02

Coeff-Com: 0.232D-02-0.822D-02 0.189D-01-0.136D-01-0.153D-01-0.503D-01

Coeff-Com: -0.614D-01 0.988D-01 0.103D+01

Coeff: -0.416D-04 0.405D-03 0.110D-02 0.162D-02 0.204D-02-0.569D-02

Coeff: 0.232D-02-0.822D-02 0.189D-01-0.136D-01-0.153D-01-0.503D-01

Coeff: -0.614D-01 0.988D-01 0.103D+01

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=2.42D-08 MaxDP=1.77D-06 DE=-9.43D-10 OVMax= 9.36D-06

Cycle 16 Pass 1 IDiag 1:

RMSU= 9.84D-09 CP: 1.00D+00 2.67D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.10D+00 2.53D+00 1.52D+00

CP: 1.05D+00 1.31D+00 1.27D+00 1.22D+00 1.35D+00

E= -1276.01357992131 Delta-E= -0.000000000070 Rises=F Damp=F

DIIS: error= 1.74D-07 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1276.01357992131 IErMin=16 ErrMin= 1.74D-07

ErrMax= 1.74D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.82D-11 BMatP= 8.46D-11

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

Coeff-Com: -0.351D-05-0.331D-03 0.185D-04 0.637D-03 0.280D-02 0.131D-02

Coeff-Com: -0.473D-02-0.851D-02 0.971D-02 0.948D-02 0.748D-02-0.383D-01

Coeff-Com: -0.132D+00-0.492D-01 0.612D+00 0.590D+00

Coeff: -0.351D-05-0.331D-03 0.185D-04 0.637D-03 0.280D-02 0.131D-02

Coeff: -0.473D-02-0.851D-02 0.971D-02 0.948D-02 0.748D-02-0.383D-01

Coeff: -0.132D+00-0.492D-01 0.612D+00 0.590D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=5.09D-08 MaxDP=1.95D-06 DE=-7.05D-11 OVMax= 4.04D-05

Cycle 17 Pass 1 IDiag 1:

RMSU= 4.04D-09 CP: 1.00D+00 2.67D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.10D+00 2.54D+00 1.53D+00

CP: 1.05D+00 1.32D+00 1.30D+00 1.28D+00 1.53D+00

CP: 9.24D-01

E= -1276.01357992135 Delta-E= -0.000000000033 Rises=F Damp=F

DIIS: error= 7.72D-08 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=17 EnMin= -1276.01357992135 IErMin=17 ErrMin= 7.72D-08

ErrMax= 7.72D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.39D-12 BMatP= 2.82D-11

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

Coeff-Com: 0.612D-05-0.239D-03-0.242D-03 0.153D-03 0.119D-02 0.171D-02

Coeff-Com: -0.353D-02-0.189D-02 0.551D-03 0.917D-02 0.657D-02-0.784D-02

Coeff-Com: -0.503D-01-0.428D-01 0.344D-01 0.278D+00 0.775D+00

Coeff: 0.612D-05-0.239D-03-0.242D-03 0.153D-03 0.119D-02 0.171D-02

Coeff: -0.353D-02-0.189D-02 0.551D-03 0.917D-02 0.657D-02-0.784D-02

Coeff: -0.503D-01-0.428D-01 0.344D-01 0.278D+00 0.775D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=8.68D-09 MaxDP=4.02D-07 DE=-3.32D-11 OVMax= 6.38D-06

Error on total polarization charges = 0.06979

SCF Done: E(UB3LYP) = -1276.01357992 A.U. after 17 cycles

NFock= 17 Conv=0.87D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7705 S= 0.5102

<L.S>= 0.000000000000E+00

KE= 1.320990148950D+03 PE=-8.598251644981D+03 EE= 3.241922094775D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.70

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7705, after 0.7503

Leave Link 502 at Tue Sep 17 13:54:26 2019, MaxMem= 2415919104 cpu: 1624.3

(Enter /home/blab/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15319 LenP2D= 41220.

LDataN: DoStor=T MaxTD1= 6 Len= 172

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

GePol: Maximum number of non-zero 1st derivatives = 241

Leave Link 701 at Tue Sep 17 13:54:29 2019, MaxMem= 2415919104 cpu: 67.6

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 13:54:29 2019, MaxMem= 2415919104 cpu: 0.3

(Enter /home/blab/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

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

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

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

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

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Tue Sep 17 13:54:42 2019, MaxMem= 2415919104 cpu: 227.6

(Enter /home/blab/g09/l716.exe)

Dipole =-2.87769808D-13-2.35811370D-13 2.22044605D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.002848537 -0.004751314 0.000000000

2 7 0.000895514 0.000700271 0.000000000

3 6 -0.006414150 -0.001104490 0.000000000

4 6 0.004062989 -0.000096556 -0.000000000

5 6 -0.001996063 0.002536267 -0.000000000

6 7 0.006759846 0.002721396 0.000000000

7 6 -0.004602532 -0.002086563 0.000000000

8 7 -0.001114711 -0.000217090 -0.000000000

9 6 -0.001644735 0.006253211 0.000000000

10 6 0.001444438 -0.004090607 0.000000000

11 6 0.003305560 0.001422913 0.000000000

12 7 -0.002168826 0.007392924 -0.000000000

13 6 -0.001444438 0.004090607 0.000000000

14 6 -0.003305560 -0.001422913 -0.000000000

15 6 0.004602532 0.002086563 0.000000000

16 7 0.001114711 0.000217090 -0.000000000

17 6 0.001644735 -0.006253211 0.000000000

18 7 -0.006759846 -0.002721396 -0.000000000

19 7 -0.000895514 -0.000700271 0.000000000

20 6 0.006414150 0.001104490 -0.000000000

21 6 -0.004062989 0.000096556 0.000000000

22 6 0.001996063 -0.002536267 -0.000000000

23 6 -0.002848537 0.004751314 -0.000000000

24 7 0.002168826 -0.007392924 -0.000000000

25 30 -0.000000000 -0.000000000 0.000000000

26 6 -0.000494404 0.000146075 -0.000000000

27 1 0.000050996 -0.000207547 0.000000000

28 6 -0.000028082 -0.000462730 -0.000000000

29 1 0.000010745 0.000170748 -0.000000000

30 6 0.000028082 0.000462730 0.000000000

31 1 -0.000010745 -0.000170748 0.000000000

32 6 0.000494404 -0.000146075 -0.000000000

33 1 -0.000050996 0.000207547 0.000000000

34 1 -0.000157641 -0.000035158 0.000000000

35 1 0.000142479 -0.000075743 0.000414953

36 1 0.000142479 -0.000075743 -0.000414953

37 1 -0.000080084 0.000250582 0.000415107

38 1 -0.000080084 0.000250582 -0.000415107

39 1 -0.000117676 -0.000147327 0.000000000

40 1 0.000080084 -0.000250582 0.000415107

41 1 0.000080084 -0.000250582 -0.000415107

42 1 0.000117676 0.000147327 0.000000000

43 1 -0.000142479 0.000075743 0.000414953

44 1 -0.000142479 0.000075743 -0.000414953

45 1 0.000157641 0.000035158 -0.000000000

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

Cartesian Forces: Max 0.007392924 RMS 0.002162439

Leave Link 716 at Tue Sep 17 13:54:42 2019, MaxMem= 2415919104 cpu: 0.3

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

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

Internal Forces: Max 0.004228182 RMS 0.000848781

Search for a local minimum.

Step number 3 out of a maximum of 270

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

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3

DE= -4.58D-04 DEPred=-2.92D-04 R= 1.57D+00

TightC=F SS= 1.41D+00 RLast= 4.55D-02 DXNew= 5.0454D-01 1.3664D-01

Trust test= 1.57D+00 RLast= 4.55D-02 DXMaxT set to 3.00D-01

ITU= 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01334

Eigenvalues --- 0.01336 0.01338 0.01339 0.01610 0.01628

Eigenvalues --- 0.01642 0.01642 0.01772 0.01789 0.01810

Eigenvalues --- 0.01811 0.01889 0.01904 0.01941 0.01944

Eigenvalues --- 0.01998 0.01999 0.02045 0.02049 0.02070

Eigenvalues --- 0.02088 0.02102 0.02112 0.02112 0.02205

Eigenvalues --- 0.02314 0.02318 0.02352 0.02374 0.06834

Eigenvalues --- 0.07159 0.07159 0.07177 0.07177 0.07239

Eigenvalues --- 0.07256 0.07275 0.07766 0.14491 0.14499

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 0.16015 0.16081

Eigenvalues --- 0.16449 0.16835 0.18508 0.22084 0.22096

Eigenvalues --- 0.23851 0.23855 0.23876 0.24108 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25246

Eigenvalues --- 0.26087 0.31443 0.33212 0.33213 0.33281

Eigenvalues --- 0.33282 0.33282 0.33367 0.33534 0.33624

Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33730 0.34137 0.34437 0.34437

Eigenvalues --- 0.34439 0.34465 0.35536 0.35541 0.35681

Eigenvalues --- 0.35682 0.35682 0.35761 0.37932 0.39009

Eigenvalues --- 0.40730 0.41663 0.41702 0.43153 0.47945

Eigenvalues --- 0.48955 0.49001 0.50081 0.51360 0.51363

Eigenvalues --- 0.51736 0.52510 0.53772 0.54005 0.54032

Eigenvalues --- 0.56321 0.56347 0.56419 1.02304

DIIS coeff's: 1.95230 -0.84084 -0.11146

Cosine: 0.997 > 0.840

Length: 0.928

GDIIS step was calculated using 3 of the last 3 vectors.

Iteration 1 RMS(Cart)= 0.00750878 RMS(Int)= 0.00003231

Iteration 2 RMS(Cart)= 0.00006514 RMS(Int)= 0.00001192

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001192

ITry= 1 IFail=0 DXMaxC= 3.21D-02 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.89D-09 for atom 29.

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

(Linear) (Quad) (Total)

R1 2.60465 -0.00035 0.00983 0.00700 0.01685 2.62149

R2 2.73045 -0.00134 -0.01062 -0.01500 -0.02563 2.70482

R3 2.53863 0.00399 0.00323 0.01441 0.01767 2.55629

R4 2.56296 -0.00027 -0.00591 -0.00505 -0.01097 2.55199

R5 3.80765 -0.00042 0.00302 0.00075 0.00377 3.81141

R6 2.76536 -0.00170 -0.00858 -0.01552 -0.02409 2.74127

R7 2.55676 0.00394 0.01225 0.02130 0.03356 2.59031

R8 2.60037 0.00228 0.00536 0.01209 0.01745 2.61782

R9 2.82223 -0.00007 0.00075 0.00034 0.00109 2.82332

R10 2.04556 0.00006 0.00020 0.00041 0.00062 2.04618

R11 2.54585 -0.00385 0.00157 -0.01081 -0.00923 2.53663

R12 2.56570 0.00017 -0.00519 -0.00370 -0.00890 2.55680

R13 2.75751 0.00228 0.00192 0.01163 0.01356 2.77106

R14 2.60443 0.00022 0.01054 0.00903 0.01953 2.62396

R15 3.80509 -0.00037 0.00133 -0.00427 -0.00298 3.80211

R16 2.76221 0.00294 -0.00508 0.00969 0.00462 2.76683

R17 2.51848 -0.00423 -0.00674 -0.01845 -0.02519 2.49329

R18 2.59096 -0.00250 -0.00099 -0.00920 -0.01016 2.58080

R19 2.81996 -0.00032 -0.00092 -0.00220 -0.00312 2.81684

R20 2.04547 -0.00014 0.00053 -0.00038 0.00016 2.04563

R21 2.51848 -0.00423 -0.00674 -0.01845 -0.02519 2.49329

R22 2.59096 -0.00250 -0.00099 -0.00920 -0.01016 2.58080

R23 2.76221 0.00294 -0.00508 0.00969 0.00462 2.76683

R24 2.81996 -0.00032 -0.00092 -0.00220 -0.00312 2.81684

R25 2.75751 0.00228 0.00192 0.01163 0.01356 2.77106

R26 2.04547 -0.00014 0.00053 -0.00038 0.00016 2.04563

R27 2.56570 0.00017 -0.00519 -0.00370 -0.00890 2.55680

R28 2.54585 -0.00385 0.00157 -0.01081 -0.00923 2.53663

R29 2.60443 0.00022 0.01054 0.00903 0.01953 2.62396

R30 3.80509 -0.00037 0.00133 -0.00427 -0.00298 3.80211

R31 2.55676 0.00394 0.01225 0.02130 0.03356 2.59031

R32 2.56296 -0.00027 -0.00591 -0.00505 -0.01097 2.55199

R33 2.60465 -0.00035 0.00983 0.00700 0.01685 2.62149

R34 3.80765 -0.00042 0.00302 0.00075 0.00377 3.81141

R35 2.76536 -0.00170 -0.00858 -0.01552 -0.02409 2.74127

R36 2.60037 0.00228 0.00536 0.01209 0.01745 2.61782

R37 2.82223 -0.00007 0.00075 0.00034 0.00109 2.82332

R38 2.73045 -0.00134 -0.01062 -0.01500 -0.02563 2.70482

R39 2.04556 0.00006 0.00020 0.00041 0.00062 2.04618

R40 2.53863 0.00399 0.00323 0.01441 0.01767 2.55629

R41 2.06403 0.00014 0.00006 0.00066 0.00072 2.06475

R42 2.06914 0.00043 -0.00162 0.00066 -0.00096 2.06819

R43 2.06914 0.00043 -0.00162 0.00066 -0.00096 2.06819

R44 2.06767 0.00046 -0.00205 0.00044 -0.00161 2.06606

R45 2.06767 0.00046 -0.00205 0.00044 -0.00161 2.06606

R46 2.06327 0.00004 -0.00047 -0.00024 -0.00072 2.06256

R47 2.06767 0.00046 -0.00205 0.00044 -0.00161 2.06606

R48 2.06767 0.00046 -0.00205 0.00044 -0.00161 2.06606

R49 2.06327 0.00004 -0.00047 -0.00024 -0.00072 2.06256

R50 2.06914 0.00043 -0.00162 0.00066 -0.00096 2.06819

R51 2.06914 0.00043 -0.00162 0.00066 -0.00096 2.06819

R52 2.06403 0.00014 0.00006 0.00066 0.00072 2.06475

A1 1.87937 0.00020 -0.00176 -0.00044 -0.00222 1.87714

A2 2.21122 -0.00085 -0.00541 -0.00841 -0.01378 2.19744

A3 2.19260 0.00064 0.00716 0.00885 0.01600 2.20860

A4 1.91365 -0.00010 -0.00126 -0.00307 -0.00433 1.90932

A5 2.18363 -0.00029 -0.00177 -0.00257 -0.00430 2.17933

A6 2.18591 0.00040 0.00303 0.00565 0.00863 2.19454

A7 1.89031 0.00068 0.00238 0.00578 0.00817 1.89848

A8 2.23201 -0.00086 0.00063 -0.00378 -0.00317 2.22884

A9 2.16086 0.00019 -0.00301 -0.00200 -0.00500 2.15586

A10 1.85824 -0.00065 -0.00027 -0.00324 -0.00350 1.85474

A11 2.17078 0.00093 0.00101 0.00621 0.00722 2.17800

A12 2.25416 -0.00028 -0.00074 -0.00297 -0.00372 2.25044

A13 1.88320 -0.00013 0.00091 0.00098 0.00188 1.88509

A14 2.17799 0.00027 0.00169 0.00326 0.00495 2.18294

A15 2.22199 -0.00015 -0.00259 -0.00424 -0.00683 2.21516

A16 2.16482 -0.00010 -0.00618 -0.00630 -0.01247 2.15234

A17 2.22428 0.00038 0.00194 0.00354 0.00550 2.22977

A18 2.17573 -0.00079 -0.00464 -0.00800 -0.01263 2.16310

A19 1.88318 0.00041 0.00270 0.00446 0.00713 1.89031

A20 1.91208 -0.00049 -0.00160 -0.00305 -0.00464 1.90745

A21 2.19397 0.00054 0.00399 0.00599 0.01002 2.20399

A22 2.17713 -0.00005 -0.00239 -0.00294 -0.00538 2.17175

A23 1.88732 -0.00012 -0.00255 -0.00242 -0.00496 1.88235

A24 2.22399 0.00026 -0.00243 -0.00067 -0.00313 2.22086

A25 2.17188 -0.00014 0.00498 0.00308 0.00809 2.17997

A26 1.85737 0.00026 0.00406 0.00392 0.00799 1.86535

A27 2.17712 -0.00012 0.00059 -0.00010 0.00048 2.17760

A28 2.24870 -0.00014 -0.00465 -0.00382 -0.00847 2.24023

A29 1.88483 -0.00005 -0.00262 -0.00291 -0.00552 1.87931

A30 2.17568 0.00013 0.00252 0.00331 0.00582 2.18150

A31 2.22268 -0.00007 0.00010 -0.00040 -0.00031 2.22237

A32 2.19421 0.00057 0.00859 0.00948 0.01808 2.21229

A33 1.85737 0.00026 0.00406 0.00392 0.00799 1.86535

A34 2.24870 -0.00014 -0.00465 -0.00382 -0.00847 2.24023

A35 2.17712 -0.00012 0.00059 -0.00010 0.00048 2.17760

A36 1.88483 -0.00005 -0.00262 -0.00291 -0.00552 1.87931

A37 2.22268 -0.00007 0.00010 -0.00040 -0.00031 2.22237

A38 2.17568 0.00013 0.00252 0.00331 0.00582 2.18150

A39 1.88318 0.00041 0.00270 0.00446 0.00713 1.89031

A40 2.17573 -0.00079 -0.00464 -0.00800 -0.01263 2.16310

A41 2.22428 0.00038 0.00194 0.00354 0.00550 2.22977

A42 1.91208 -0.00049 -0.00160 -0.00305 -0.00464 1.90745

A43 2.19397 0.00054 0.00399 0.00599 0.01002 2.20399

A44 2.17713 -0.00005 -0.00239 -0.00294 -0.00538 2.17175

A45 2.17188 -0.00014 0.00498 0.00308 0.00809 2.17997

A46 2.22399 0.00026 -0.00243 -0.00067 -0.00313 2.22086

A47 1.88732 -0.00012 -0.00255 -0.00242 -0.00496 1.88235

A48 2.16482 -0.00010 -0.00618 -0.00630 -0.01247 2.15234

A49 1.91365 -0.00010 -0.00126 -0.00307 -0.00433 1.90932

A50 2.18591 0.00040 0.00303 0.00565 0.00863 2.19454

A51 2.18363 -0.00029 -0.00177 -0.00257 -0.00430 2.17933

A52 2.23201 -0.00086 0.00063 -0.00378 -0.00317 2.22884

A53 2.16086 0.00019 -0.00301 -0.00200 -0.00500 2.15586

A54 1.89031 0.00068 0.00238 0.00578 0.00817 1.89848

A55 1.85824 -0.00065 -0.00027 -0.00324 -0.00350 1.85474

A56 2.17078 0.00093 0.00101 0.00621 0.00722 2.17800

A57 2.25416 -0.00028 -0.00074 -0.00297 -0.00372 2.25044

A58 1.88320 -0.00013 0.00091 0.00098 0.00188 1.88509

A59 2.22199 -0.00015 -0.00259 -0.00424 -0.00683 2.21516

A60 2.17799 0.00027 0.00169 0.00326 0.00495 2.18294

A61 1.87937 0.00020 -0.00176 -0.00044 -0.00222 1.87714

A62 2.21122 -0.00085 -0.00541 -0.00841 -0.01378 2.19744

A63 2.19260 0.00064 0.00716 0.00885 0.01600 2.20860

A64 2.19421 0.00057 0.00859 0.00948 0.01808 2.21229

A65 1.56539 -0.00036 -0.00341 -0.00510 -0.00850 1.55689

A66 1.57620 0.00036 0.00341 0.00510 0.00850 1.58470

A67 1.57620 0.00036 0.00341 0.00510 0.00850 1.58470

A68 1.56539 -0.00036 -0.00341 -0.00510 -0.00850 1.55689

A69 1.94514 -0.00012 0.00347 0.00088 0.00433 1.94947

A70 1.94692 -0.00002 0.00286 0.00253 0.00536 1.95228

A71 1.94692 -0.00002 0.00286 0.00253 0.00536 1.95228

A72 1.88322 0.00002 -0.00265 -0.00246 -0.00513 1.87809

A73 1.88322 0.00002 -0.00265 -0.00246 -0.00513 1.87809

A74 1.85436 0.00013 -0.00454 -0.00140 -0.00596 1.84840

A75 1.94351 -0.00018 0.00135 -0.00075 0.00060 1.94411

A76 1.94351 -0.00018 0.00135 -0.00075 0.00060 1.94411

A77 1.94474 -0.00017 0.00243 0.00034 0.00277 1.94751

A78 1.85727 0.00018 -0.00335 -0.00115 -0.00450 1.85277

A79 1.88560 0.00019 -0.00107 0.00118 0.00009 1.88570

A80 1.88560 0.00019 -0.00107 0.00118 0.00009 1.88570

A81 1.94351 -0.00018 0.00135 -0.00075 0.00060 1.94411

A82 1.94351 -0.00018 0.00135 -0.00075 0.00060 1.94411

A83 1.94474 -0.00017 0.00243 0.00034 0.00277 1.94751

A84 1.85727 0.00018 -0.00335 -0.00115 -0.00450 1.85277

A85 1.88560 0.00019 -0.00107 0.00118 0.00009 1.88570

A86 1.88560 0.00019 -0.00107 0.00118 0.00009 1.88570

A87 1.94692 -0.00002 0.00286 0.00253 0.00536 1.95228

A88 1.94692 -0.00002 0.00286 0.00253 0.00536 1.95228

A89 1.94514 -0.00012 0.00347 0.00088 0.00433 1.94947

A90 1.85436 0.00013 -0.00454 -0.00140 -0.00596 1.84840

A91 1.88322 0.00002 -0.00265 -0.00246 -0.00513 1.87809

A92 1.88322 0.00002 -0.00265 -0.00246 -0.00513 1.87809

A93 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

A94 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

A95 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

A96 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D1 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D2 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D3 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D4 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D5 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D6 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D7 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D8 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D10 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D11 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D12 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D13 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D14 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D15 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D16 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D17 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D18 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D19 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D20 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D21 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D22 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D23 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D24 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D25 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D26 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D27 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D28 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D29 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D30 1.03537 0.00007 -0.00097 0.00079 -0.00018 1.03519

D31 -1.03537 -0.00007 0.00097 -0.00079 0.00018 -1.03519

D32 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D33 -2.10623 0.00007 -0.00097 0.00079 -0.00018 -2.10640

D34 2.10623 -0.00007 0.00097 -0.00079 0.00018 2.10640

D35 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D36 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D37 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D38 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D39 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D40 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D41 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D42 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D43 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D44 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D45 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D46 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D47 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D48 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D49 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D50 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D51 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D52 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D53 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D54 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D55 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D56 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D57 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D58 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D59 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D60 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D61 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D62 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D63 1.03495 -0.00001 -0.00122 -0.00122 -0.00244 1.03251

D64 -1.03495 0.00001 0.00122 0.00122 0.00244 -1.03251

D65 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D66 -2.10664 -0.00001 -0.00122 -0.00122 -0.00244 -2.10908

D67 2.10664 0.00001 0.00122 0.00122 0.00244 2.10908

D68 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D69 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D70 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D71 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D72 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D73 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D74 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D75 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D76 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D77 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D78 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D79 -2.10664 -0.00001 -0.00122 -0.00122 -0.00244 -2.10908

D80 2.10664 0.00001 0.00122 0.00122 0.00244 2.10908

D81 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D82 1.03495 -0.00001 -0.00122 -0.00122 -0.00244 1.03251

D83 -1.03495 0.00001 0.00122 0.00122 0.00244 -1.03251

D84 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D85 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D86 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D87 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D88 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D89 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D90 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D91 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D92 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D93 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D94 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D95 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D96 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D97 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D98 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D99 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D100 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D101 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D102 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D103 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D104 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D105 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D106 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D107 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D108 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D109 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D110 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D111 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D112 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D113 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D114 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D115 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D116 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D117 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D118 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D119 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D120 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D121 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D122 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D123 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D124 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D125 1.03537 0.00007 -0.00097 0.00079 -0.00018 1.03519

D126 -1.03537 -0.00007 0.00097 -0.00079 0.00018 -1.03519

D127 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D128 -2.10623 0.00007 -0.00097 0.00079 -0.00018 -2.10640

D129 2.10623 -0.00007 0.00097 -0.00079 0.00018 2.10640

D130 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D131 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D132 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D133 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D134 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D135 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D136 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

Item Value Threshold Converged?

Maximum Force 0.004228 0.000450 NO

RMS Force 0.000849 0.000300 NO

Maximum Displacement 0.032090 0.001800 NO

RMS Displacement 0.007480 0.001200 NO

Predicted change in Energy=-6.564642D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 13:54:42 2019, MaxMem= 2415919104 cpu: 1.4

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

Input orientation:

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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1 6 0 -2.086020 -2.199956 -0.000000

2 7 0 -0.736778 -1.877524 -0.000000

3 6 0 -0.004506 -3.012208 -0.000000

4 6 0 -0.905329 -4.149226 -0.000000

5 6 0 -2.188662 -3.627601 -0.000000

6 7 0 1.361287 -3.128504 -0.000000

7 6 0 2.191154 -2.073441 -0.000000

8 7 0 1.862542 -0.760952 -0.000000

9 6 0 3.022496 0.002299 -0.000000

10 6 0 4.163494 -0.915220 -0.000000

11 6 0 3.653505 -2.182122 -0.000000

12 7 0 -3.112255 -1.318635 -0.000000

13 6 0 -4.163494 0.915220 -0.000000

14 6 0 -3.653505 2.182122 -0.000000

15 6 0 -2.191154 2.073441 -0.000000

16 7 0 -1.862542 0.760952 -0.000000

17 6 0 -3.022496 -0.002299 -0.000000

18 7 0 -1.361287 3.128504 -0.000000

19 7 0 0.736778 1.877524 -0.000000

20 6 0 0.004506 3.012208 -0.000000

21 6 0 0.905329 4.149226 -0.000000

22 6 0 2.188662 3.627601 -0.000000

23 6 0 2.086020 2.199956 -0.000000

24 7 0 3.112255 1.318635 -0.000000

25 30 0 0.000000 -0.000000 -0.000000

26 6 0 -0.472977 -5.579338 -0.000000

27 1 0 -3.117173 -4.184646 -0.000000

28 6 0 5.593242 -0.493642 -0.000000

29 1 0 4.206824 -3.112523 -0.000000

30 6 0 -5.593242 0.493642 -0.000000

31 1 0 -4.206824 3.112523 -0.000000

32 6 0 0.472977 5.579338 -0.000000

33 1 0 3.117173 4.184646 -0.000000

34 1 0 -1.327858 -6.259774 -0.000000

35 1 0 0.141161 -5.819342 0.873513

36 1 0 0.141161 -5.819342 -0.873513

37 1 0 5.828087 0.119716 0.874051

38 1 0 5.828087 0.119716 -0.874051

39 1 0 6.265402 -1.353573 -0.000000

40 1 0 -5.828087 -0.119716 0.874051

41 1 0 -5.828087 -0.119716 -0.874051

42 1 0 -6.265402 1.353573 -0.000000

43 1 0 -0.141161 5.819342 0.873513

44 1 0 -0.141161 5.819342 -0.873513

45 1 0 1.327858 6.259774 -0.000000

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Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.387233 0.000000

3 C 2.234380 1.350456 0.000000

4 C 2.278965 2.277946 1.450618 0.000000

5 C 1.431329 2.273925 2.269195 1.385293 0.000000

6 N 3.570172 2.442709 1.370735 2.485844 3.584862

7 C 4.279045 2.934480 2.387929 3.727880 4.647386

8 N 4.202603 2.828992 2.924726 4.375101 4.962855

9 C 5.562991 4.203080 4.272001 5.715153 6.350775

10 C 6.380202 4.993866 4.665789 6.012633 6.907018

11 C 5.739553 4.400837 3.751011 4.965125 6.018332

12 N 1.352732 2.440337 3.539250 3.589257 2.486835

13 C 3.744358 4.420610 5.720303 6.021980 4.953501

14 C 4.653990 4.998802 6.347933 6.902060 5.991548

15 C 4.274690 4.210146 5.535815 6.354127 5.701042

16 N 2.969330 2.868606 4.205833 5.002609 4.400653

17 C 2.388867 2.956514 4.262372 4.656114 3.719959

18 N 5.377520 5.044831 6.288815 7.291998 6.806577

19 N 4.959237 4.033826 4.945602 6.246457 6.234148

20 C 5.615777 4.945602 6.024422 7.218998 6.992642

21 C 7.018567 6.246457 7.218998 8.493690 8.369696

22 C 7.227263 6.234148 6.992642 8.369696 8.473424

23 C 6.063427 4.959237 5.615777 7.018567 7.227263

24 N 6.277145 5.003047 5.335766 6.785166 7.250170

25 Zn 3.031714 2.016913 3.012211 4.246845 4.236712

26 C 3.744614 3.711202 2.609526 1.494038 2.598625

27 H 2.236576 3.314980 3.326155 2.212128 1.082790

28 C 7.866548 6.479528 6.138237 7.456186 8.389262

29 H 6.358669 5.095530 4.212525 5.216212 6.416194

30 C 4.422225 5.404412 6.597344 6.597935 5.345635

31 H 5.720161 6.077975 7.427772 7.977021 7.035783

32 C 8.189377 7.554356 8.604804 9.825715 9.583947

33 H 8.236284 7.183512 7.844717 9.253861 9.443680

34 H 4.130004 4.421933 3.506843 2.152428 2.769354

35 H 4.338585 4.131796 2.943510 2.155796 3.315845

36 H 4.338585 4.131796 2.943510 2.155796 3.315845

37 H 8.293246 6.917397 6.677728 8.020394 8.892390

38 H 8.293246 6.917397 6.677728 8.020394 8.892390

39 H 8.394202 7.021756 6.485586 7.696432 8.754565

40 H 4.369717 5.456672 6.560835 6.421406 5.129779

41 H 4.369717 5.456672 6.560835 6.421406 5.129779

42 H 5.485873 6.403567 7.632749 7.681873 6.436762

43 H 8.297870 7.769140 8.875696 10.035902 9.705669

44 H 8.297870 7.769140 8.875696 10.035902 9.705669

45 H 9.122587 8.395138 9.367221 10.645863 10.494098

6 7 8 9 10

6 N 0.000000

7 C 1.342325 0.000000

8 N 2.420033 1.353001 0.000000

9 C 3.544227 2.236029 1.388541 0.000000

10 C 3.570853 2.287269 2.306118 1.464143 0.000000

11 C 2.479900 1.466384 2.286323 2.273734 1.365698

12 N 4.825785 5.356853 5.005957 6.275351 7.286924

13 C 6.846524 7.022367 6.254811 7.243747 8.525798

14 C 7.304169 7.229789 6.252076 7.022864 8.408269

15 C 6.299211 6.033345 4.946335 5.609971 7.022367

16 N 5.051825 4.946335 4.023983 4.943597 6.254811

17 C 5.384302 5.609971 4.943597 6.044994 7.243747

18 N 6.823676 6.299211 5.051825 5.384302 6.846524

19 N 5.044831 4.210146 2.868606 2.956514 4.420610

20 C 6.288815 5.535815 4.205833 4.262372 5.720303

21 C 7.291998 6.354127 5.002609 4.656114 6.021980

22 C 6.806577 5.701042 4.400653 3.719959 4.953501

23 C 5.377520 4.274690 2.969330 2.388867 3.744358

24 N 4.779428 3.514912 2.426204 1.319392 2.468848

25 Zn 3.411838 3.016672 2.011992 3.022497 4.262899

26 C 3.061228 4.403284 5.354577 6.585819 6.576539

27 H 4.601309 5.712751 6.043116 7.431423 7.981057

28 C 4.985172 3.750996 3.740264 2.618146 1.490606

29 H 2.845582 2.267734 3.320474 3.332379 2.197731

30 C 7.841263 8.196751 7.560603 8.629737 9.857930

31 H 8.363867 8.235796 7.200070 7.869979 9.288968

32 C 8.753034 7.843288 6.490776 6.132162 7.469886

33 H 7.520991 6.326229 5.102259 4.183419 5.206094

34 H 4.127512 5.468896 6.357334 7.624902 7.662846

35 H 3.080965 4.358586 5.414193 6.554130 6.402547

36 H 3.080965 4.358586 5.414193 6.554130 6.402547

37 H 5.591708 4.336033 4.155128 2.940933 2.146142

38 H 5.591708 4.336033 4.155128 2.940933 2.146142

39 H 5.215432 4.137356 4.442565 3.514943 2.147131

40 H 7.842440 8.299953 7.766654 8.894474 10.061236

41 H 7.842440 8.299953 7.766654 8.894474 10.061236

42 H 8.846208 9.124569 8.398493 9.385681 10.672830

43 H 9.115060 8.276397 6.933839 6.679053 8.040361

44 H 9.115060 8.276397 6.933839 6.679053 8.040361

45 H 9.388337 8.377813 7.041057 6.482885 7.715009

11 12 13 14 15

11 C 0.000000

12 N 6.820639 0.000000

13 C 8.408269 2.468848 0.000000

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16 N 6.252076 2.426204 2.306118 2.286323 1.353001

17 C 7.022864 1.319392 1.464143 2.273734 2.236029

18 N 7.304169 4.779428 3.570853 2.479900 1.342325

19 N 4.998802 5.003047 4.993866 4.400837 2.934480

20 C 6.347933 5.335766 4.665789 3.751011 2.387929

21 C 6.902060 6.785166 6.012633 4.965125 3.727880

22 C 5.991548 7.250170 6.907018 6.018332 4.647386

23 C 4.653990 6.277145 6.380202 5.739553 4.279045

24 N 3.542351 6.760156 7.286924 6.820639 5.356853

25 Zn 4.255556 3.380078 4.262899 4.255556 3.016672

26 C 5.344991 5.011924 7.469886 8.387850 7.843288

27 H 7.060608 2.866016 5.206094 6.389319 6.326229

28 C 2.571681 8.744500 9.857930 9.626112 8.196751

29 H 1.082501 7.535712 9.288968 9.477238 8.235796

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32 C 8.387850 7.774054 6.576539 5.344991 4.403284

33 H 6.389319 8.312152 7.981057 7.060608 5.712751

34 H 6.437485 5.253468 7.715009 8.756383 8.377813

35 H 5.131175 5.621753 8.040361 8.898649 8.276397

36 H 5.131175 5.621753 8.040361 8.898649 8.276397

37 H 3.285001 9.097391 10.061236 9.742590 8.299953

38 H 3.285001 9.097391 10.061236 9.742590 8.299953

39 H 2.740165 9.377722 10.672830 10.530235 9.124569

40 H 9.742590 3.094691 2.146142 3.285001 4.336033

41 H 9.742590 3.094691 2.146142 3.285001 4.336033

42 H 10.530235 4.133163 2.147131 2.740165 4.137356

43 H 8.898649 7.780819 6.402547 5.131175 4.358586

44 H 8.898649 7.780819 6.402547 5.131175 4.358586

45 H 8.756383 8.783329 7.662846 6.437485 5.468896

16 17 18 19 20

16 N 0.000000

17 C 1.388541 0.000000

18 N 2.420033 3.544227 0.000000

19 N 2.828992 4.203080 2.442709 0.000000

20 C 2.924726 4.272001 1.370735 1.350456 0.000000

21 C 4.375101 5.715153 2.485844 2.277946 1.450618

22 C 4.962855 6.350775 3.584862 2.273925 2.269195

23 C 4.202603 5.562991 3.570172 1.387233 2.234380

24 N 5.005957 6.275351 4.825785 2.440337 3.539250

25 Zn 2.011992 3.022497 3.411838 2.016913 3.012211

26 C 6.490776 6.132162 8.753034 7.554356 8.604804

27 H 5.102259 4.183419 7.520991 7.183512 7.844717

28 C 7.560603 8.629737 7.841263 5.404412 6.597344

29 H 7.200070 7.869979 8.363867 6.077975 7.427772

30 C 3.740264 2.618146 4.985172 6.479528 6.138237

31 H 3.320474 3.332379 2.845582 5.095530 4.212525

32 C 5.354577 6.585819 3.061228 3.711202 2.609526

33 H 6.043116 7.431423 4.601309 3.314980 3.326155

34 H 7.041057 6.482885 9.388337 8.395138 9.367221

35 H 6.933839 6.679053 9.115060 7.769140 8.875696

36 H 6.933839 6.679053 9.115060 7.769140 8.875696

37 H 7.766654 8.894474 7.842440 5.456672 6.560835

38 H 7.766654 8.894474 7.842440 5.456672 6.560835

39 H 8.398493 9.385681 8.846208 6.403567 7.632749

40 H 4.155128 2.940933 5.591708 6.917397 6.677728

41 H 4.155128 2.940933 5.591708 6.917397 6.677728

42 H 4.442565 3.514943 5.215432 7.021756 6.485586

43 H 5.414193 6.554130 3.080965 4.131796 2.943510

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45 H 6.357334 7.624902 4.127512 4.421933 3.506843

21 22 23 24 25

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22 C 1.385293 0.000000

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28 C 6.597935 5.345635 4.422225 3.072401 5.614983

29 H 7.977021 7.035783 5.720161 4.564345 5.233084

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32 C 1.494038 2.598625 3.744614 5.011924 5.599350

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35 H 10.035902 9.705669 8.297870 7.780819 5.886229

36 H 10.035902 9.705669 8.297870 7.780819 5.886229

37 H 6.421406 5.129779 4.369717 3.094691 5.894480

38 H 6.421406 5.129779 4.369717 3.094691 5.894480

39 H 7.681873 6.436762 5.485873 4.133163 6.409947

40 H 8.020394 8.892390 8.293246 9.097391 5.894480

41 H 8.020394 8.892390 8.293246 9.097391 5.894480

42 H 7.696432 8.754565 8.394202 9.377722 6.409947

43 H 2.155796 3.315845 4.338585 5.621753 5.886229

44 H 2.155796 3.315845 4.338585 5.621753 5.886229

45 H 2.152428 2.769354 4.130004 5.253468 6.399061

26 27 28 29 30

26 C 0.000000

27 H 2.989471 0.000000

28 C 7.916017 9.460172 0.000000

29 H 5.290153 7.402053 2.963223 0.000000

30 C 7.943438 5.293137 11.229967 10.442496 0.000000

31 H 9.459919 7.378077 10.442496 10.466168 2.963223

32 C 11.198701 10.403104 7.943438 9.459919 7.916017

33 H 10.403104 10.436098 5.293137 7.378077 9.460172

34 H 1.092618 2.740037 9.008324 6.366937 7.987624

35 H 1.094437 3.748600 7.671459 4.961805 8.573224

36 H 1.094437 3.748600 7.671459 4.961805 8.573224

37 H 8.540878 9.965399 1.093310 3.720192 11.460826

38 H 8.540878 9.965399 1.093310 3.720192 11.460826

39 H 7.953795 9.800393 1.091458 2.707702 12.001652

40 H 7.697314 4.963534 11.460826 10.508106 1.093310

41 H 7.697314 4.963534 11.460826 10.508106 1.093310

42 H 9.034237 6.370496 12.001652 11.384794 1.091458

43 H 11.436916 10.473751 8.573224 9.972272 7.671459

44 H 11.436916 10.473751 8.573224 9.972272 7.671459

45 H 11.975291 11.350957 7.987624 9.804509 9.008324

31 32 33 34 35

31 H 0.000000

32 C 5.290153 0.000000

33 H 7.402053 2.989471 0.000000

34 H 9.804509 11.975291 11.350957 0.000000

35 H 9.972272 11.436916 10.473751 1.764943 0.000000

36 H 9.972272 11.436916 10.473751 1.764943 1.747027

37 H 10.508106 7.697314 4.963534 9.626495 8.222745

38 H 10.508106 7.697314 4.963534 9.626495 8.406397

39 H 11.384794 9.034237 6.370496 9.040377 7.629709

40 H 3.720192 8.540878 9.965399 7.662658 8.253342

41 H 3.720192 8.540878 9.965399 7.662658 8.436328

42 H 2.707702 7.953795 9.800393 9.074271 9.657007

43 H 4.961805 1.094437 3.748600 12.168661 11.642108

44 H 4.961805 1.094437 3.748600 12.168661 11.772459

45 H 6.366937 1.092618 2.740037 12.798121 12.168661

36 37 38 39 40

36 H 0.000000

37 H 8.406397 0.000000

38 H 8.222745 1.748102 0.000000

39 H 7.629709 1.767990 1.767990 0.000000

40 H 8.436328 11.658632 11.788959 12.187651 0.000000

41 H 8.253342 11.788959 11.658632 12.187651 1.748102

42 H 9.657007 12.187651 12.187651 12.819895 1.767990

43 H 11.772459 8.253342 8.436328 9.657007 8.222745

44 H 11.642108 8.436328 8.253342 9.657007 8.406397

45 H 12.168661 7.662658 7.662658 9.074271 9.626495

41 42 43 44 45

41 H 0.000000

42 H 1.767990 0.000000

43 H 8.406397 7.629709 0.000000

44 H 8.222745 7.629709 1.747027 0.000000

45 H 9.626495 9.040377 1.764943 1.764943 0.000000

Stoichiometry C20H16N8Zn(1-,2)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=3 Diff= 2.19D-01

Largest Abelian subgroup C2H NOp 4

Largest concise Abelian subgroup C2H 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 -2.958368 0.662830 0.000000

2 7 0 -1.989701 -0.330195 0.000000

3 6 0 -2.588369 -1.540702 0.000000

4 6 0 -4.026443 -1.350351 0.000000

5 6 0 -4.236670 0.018897 0.000000

6 7 0 -1.987874 -2.772903 0.000000

7 6 0 -0.656544 -2.944361 0.000000

8 7 0 0.301759 -1.989234 0.000000

9 6 0 1.551820 -2.593712 0.000000

10 6 0 1.349176 -4.043764 0.000000

11 6 0 0.000000 -4.255556 0.000000

12 7 0 -2.727954 1.995795 0.000000

13 6 0 -1.349176 4.043764 0.000000

14 6 0 0.000000 4.255556 0.000000

15 6 0 0.656544 2.944361 0.000000

16 7 0 -0.301759 1.989234 0.000000

17 6 0 -1.551820 2.593712 0.000000

18 7 0 1.987874 2.772903 0.000000

19 7 0 1.989701 0.330195 0.000000

20 6 0 2.588369 1.540702 0.000000

21 6 0 4.026443 1.350351 0.000000

22 6 0 4.236670 -0.018897 0.000000

23 6 0 2.958368 -0.662830 0.000000

24 7 0 2.727954 -1.995795 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -5.032535 -2.454855 0.000000

27 1 0 -5.191021 0.530412 0.000000

28 6 0 2.444243 -5.055068 0.000000

29 1 0 -0.515048 -5.207677 0.000000

30 6 0 -2.444243 5.055068 0.000000

31 1 0 0.515048 5.207677 0.000000

32 6 0 5.032535 2.454855 0.000000

33 1 0 5.191021 -0.530412 0.000000

34 1 0 -6.055064 -2.069825 0.000000

35 1 0 -4.923673 -3.105176 0.873513

36 1 0 -4.923673 -3.105176 -0.873513

37 1 0 3.091249 -4.942176 0.874051

38 1 0 3.091249 -4.942176 -0.874051

39 1 0 2.050635 -6.073082 0.000000

40 1 0 -3.091249 4.942176 0.874051

41 1 0 -3.091249 4.942176 -0.874051

42 1 0 -2.050635 6.073082 0.000000

43 1 0 4.923673 3.105176 0.873513

44 1 0 4.923673 3.105176 -0.873513

45 1 0 6.055064 2.069825 0.000000

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

Rotational constants (GHZ): 0.1827179 0.1812509 0.0911929

Leave Link 202 at Tue Sep 17 13:54:42 2019, MaxMem= 2415919104 cpu: 0.2

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 229 symmetry adapted cartesian basis functions of AG symmetry.

There are 82 symmetry adapted cartesian basis functions of BG symmetry.

There are 78 symmetry adapted cartesian basis functions of AU symmetry.

There are 218 symmetry adapted cartesian basis functions of BU symmetry.

There are 212 symmetry adapted basis functions of AG symmetry.

There are 82 symmetry adapted basis functions of BG symmetry.

There are 78 symmetry adapted basis functions of AU symmetry.

There are 204 symmetry adapted basis functions of BU symmetry.

576 basis functions, 1015 primitive gaussians, 607 cartesian basis functions

103 alpha electrons 102 beta electrons

nuclear repulsion energy 2758.5386486950 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= 45 NActive= 45 NUniq= 21 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1141078621 Hartrees.

Nuclear repulsion after empirical dispersion term = 2758.4245408329 Hartrees.

No density basis found on file 724.

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

Polarizable Continuum Model (PCM)

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

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

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 = 45

GePol: Total number of spheres = 45

GePol: Number of exposed spheres = 45 (100.00%)

GePol: Number of points = 3598

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.28D-09

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 258

GePol: Fraction of low-weight points (<1% of avg) = 7.17%

GePol: Cavity surface area = 378.966 Ang\*\*2

GePol: Cavity volume = 378.228 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0106345458 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2758.4139062872 Hartrees.

Leave Link 301 at Tue Sep 17 13:54:42 2019, MaxMem= 2415919104 cpu: 1.6

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15305 LenP2D= 41192.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.78D-04 NBF= 212 82 78 204

NBsUse= 576 1.00D-06 EigRej= -1.00D+00 NBFU= 212 82 78 204

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= 594 594 594 594 594 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Tue Sep 17 13:54:43 2019, MaxMem= 2415919104 cpu: 10.4

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 13:54:43 2019, MaxMem= 2415919104 cpu: 1.2

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

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

B after Tr= -0.000000 -0.000000 -0.000000

Rot= 0.997007 -0.000000 0.000000 -0.077314 Ang= -8.87 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-BG.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7706 S= 0.5102

Generating alternative initial guess.

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -1276.41170953137

Leave Link 401 at Tue Sep 17 13:54:45 2019, MaxMem= 2415919104 cpu: 40.0

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1141655 IEndB= 1141655 NGot= 2415919104 MDV= 2415163146

LenX= 2415163146 LenY= 2414794090

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= 670000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 38836812.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.44D-15 for 3585.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.22D-15 for 3594 1327.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.55D-15 for 3585.

Iteration 1 A^-1\*A deviation from orthogonality is 2.32D-11 for 1727 1721.

E= -1276.01128499381

DIIS: error= 1.62D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1276.01128499381 IErMin= 1 ErrMin= 1.62D-03

ErrMax= 1.62D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.79D-03 BMatP= 4.79D-03

IDIUse=3 WtCom= 9.84D-01 WtEn= 1.62D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.292 Goal= None Shift= 0.000

Gap= 0.343 Goal= None Shift= 0.000

GapD= 0.292 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.

RMSDP=1.24D-04 MaxDP=3.20D-03 OVMax= 6.49D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.24D-04 CP: 1.00D+00

E= -1276.01314176045 Delta-E= -0.001856766640 Rises=F Damp=F

DIIS: error= 1.01D-03 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1276.01314176045 IErMin= 2 ErrMin= 1.01D-03

ErrMax= 1.01D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.38D-04 BMatP= 4.79D-03

IDIUse=3 WtCom= 9.90D-01 WtEn= 1.01D-02

Coeff-Com: 0.166D+00 0.834D+00

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

Coeff: 0.165D+00 0.835D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=5.15D-05 MaxDP=2.63D-03 DE=-1.86D-03 OVMax= 1.96D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 4.90D-05 CP: 1.00D+00 1.13D+00

E= -1276.01316696162 Delta-E= -0.000025201171 Rises=F Damp=F

DIIS: error= 1.58D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1276.01316696162 IErMin= 2 ErrMin= 1.01D-03

ErrMax= 1.58D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.09D-03 BMatP= 8.38D-04

IDIUse=3 WtCom= 2.01D-01 WtEn= 7.99D-01

Coeff-Com: -0.542D-02 0.537D+00 0.468D+00

Coeff-En: 0.000D+00 0.472D+00 0.528D+00

Coeff: -0.109D-02 0.485D+00 0.516D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=5.02D-05 MaxDP=2.13D-03 DE=-2.52D-05 OVMax= 2.99D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 3.79D-05 CP: 1.00D+00 1.33D+00 5.82D-01

E= -1276.01345353153 Delta-E= -0.000286569908 Rises=F Damp=F

DIIS: error= 7.69D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1276.01345353153 IErMin= 4 ErrMin= 7.69D-04

ErrMax= 7.69D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.43D-04 BMatP= 8.38D-04

IDIUse=3 WtCom= 9.92D-01 WtEn= 7.69D-03

Coeff-Com: -0.957D-02 0.899D-01 0.337D+00 0.583D+00

Coeff-En: 0.000D+00 0.000D+00 0.753D-01 0.925D+00

Coeff: -0.950D-02 0.892D-01 0.335D+00 0.586D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=2.44D-05 MaxDP=7.85D-04 DE=-2.87D-04 OVMax= 1.66D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 9.14D-06 CP: 1.00D+00 1.43D+00 9.30D-01 1.24D+00

E= -1276.01355459884 Delta-E= -0.000101067314 Rises=F Damp=F

DIIS: error= 3.82D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1276.01355459884 IErMin= 5 ErrMin= 3.82D-04

ErrMax= 3.82D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.31D-05 BMatP= 2.43D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.82D-03

Coeff-Com: -0.357D-02-0.268D-01 0.186D+00 0.348D+00 0.496D+00

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

Coeff: -0.356D-02-0.267D-01 0.185D+00 0.347D+00 0.498D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=1.64D-05 MaxDP=6.33D-04 DE=-1.01D-04 OVMax= 1.29D-02

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.45D-06 CP: 1.00D+00 1.50D+00 1.05D+00 1.53D+00 1.19D+00

E= -1276.01359203019 Delta-E= -0.000037431346 Rises=F Damp=F

DIIS: error= 3.39D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1276.01359203019 IErMin= 6 ErrMin= 3.39D-04

ErrMax= 3.39D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.87D-05 BMatP= 3.31D-05

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.39D-03

Coeff-Com: 0.892D-02-0.120D+00-0.119D+00-0.391D+00-0.135D+00 0.175D+01

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

Coeff: 0.889D-02-0.119D+00-0.118D+00-0.390D+00-0.134D+00 0.175D+01

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=5.07D-05 MaxDP=1.87D-03 DE=-3.74D-05 OVMax= 4.04D-02

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.08D-06 CP: 1.00D+00 1.74D+00 1.48D+00 2.39D+00 2.48D+00

CP: 2.73D+00

E= -1276.01367357580 Delta-E= -0.000081545613 Rises=F Damp=F

DIIS: error= 1.78D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1276.01367357580 IErMin= 7 ErrMin= 1.78D-04

ErrMax= 1.78D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.69D-06 BMatP= 1.87D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.78D-03

Coeff-Com: 0.532D-02-0.347D-01-0.104D+00-0.364D+00-0.451D+00 0.844D+00

Coeff-Com: 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: 0.100D+01

Coeff: 0.531D-02-0.347D-01-0.104D+00-0.364D+00-0.450D+00 0.842D+00

Coeff: 0.110D+01

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=4.01D-05 MaxDP=1.59D-03 DE=-8.15D-05 OVMax= 3.18D-02

Cycle 8 Pass 1 IDiag 1:

RMSU= 8.93D-06 CP: 1.00D+00 1.92D+00 1.81D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.98D+00

E= -1276.01370759538 Delta-E= -0.000034019579 Rises=F Damp=F

DIIS: error= 8.95D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1276.01370759538 IErMin= 8 ErrMin= 8.95D-05

ErrMax= 8.95D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.30D-06 BMatP= 7.69D-06

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

Coeff-Com: -0.352D-02 0.793D-01 0.808D-01 0.126D+00-0.135D+00-0.774D+00

Coeff-Com: 0.700D+00 0.926D+00

Coeff: -0.352D-02 0.793D-01 0.808D-01 0.126D+00-0.135D+00-0.774D+00

Coeff: 0.700D+00 0.926D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.56D-05 MaxDP=7.10D-04 DE=-3.40D-05 OVMax= 1.22D-02

Cycle 9 Pass 1 IDiag 1:

RMSU= 7.96D-06 CP: 1.00D+00 1.99D+00 1.93D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.66D+00 1.91D+00

E= -1276.01371474457 Delta-E= -0.000007149190 Rises=F Damp=F

DIIS: error= 4.28D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1276.01371474457 IErMin= 9 ErrMin= 4.28D-05

ErrMax= 4.28D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.54D-07 BMatP= 3.30D-06

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

Coeff-Com: -0.270D-02 0.345D-01 0.507D-01 0.119D+00 0.417D-01-0.492D+00

Coeff-Com: 0.466D-02 0.374D+00 0.870D+00

Coeff: -0.270D-02 0.345D-01 0.507D-01 0.119D+00 0.417D-01-0.492D+00

Coeff: 0.466D-02 0.374D+00 0.870D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=9.21D-06 MaxDP=4.02D-04 DE=-7.15D-06 OVMax= 7.14D-03

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.25D-06 CP: 1.00D+00 2.02D+00 2.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.46D+00 1.56D+00

E= -1276.01371648792 Delta-E= -0.000001743351 Rises=F Damp=F

DIIS: error= 2.78D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1276.01371648792 IErMin=10 ErrMin= 2.78D-05

ErrMax= 2.78D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.61D-07 BMatP= 7.54D-07

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

Coeff-Com: -0.384D-03-0.698D-02 0.156D-01 0.594D-01 0.108D+00-0.340D-01

Coeff-Com: -0.331D+00-0.112D+00 0.516D+00 0.786D+00

Coeff: -0.384D-03-0.698D-02 0.156D-01 0.594D-01 0.108D+00-0.340D-01

Coeff: -0.331D+00-0.112D+00 0.516D+00 0.786D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=1.28D-06 MaxDP=6.55D-05 DE=-1.74D-06 OVMax= 4.42D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.23D-06 CP: 1.00D+00 2.02D+00 2.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.48D+00 1.56D+00 8.17D-01

E= -1276.01371670098 Delta-E= -0.000000213064 Rises=F Damp=F

DIIS: error= 1.37D-05 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1276.01371670098 IErMin=11 ErrMin= 1.37D-05

ErrMax= 1.37D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.63D-07 BMatP= 3.61D-07

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

Coeff-Com: 0.542D-03-0.133D-01-0.972D-02-0.116D-01 0.166D-01 0.115D+00

Coeff-Com: -0.146D+00-0.919D-01-0.139D-01 0.477D+00 0.676D+00

Coeff: 0.542D-03-0.133D-01-0.972D-02-0.116D-01 0.166D-01 0.115D+00

Coeff: -0.146D+00-0.919D-01-0.139D-01 0.477D+00 0.676D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=2.84D-06 MaxDP=1.10D-04 DE=-2.13D-07 OVMax= 2.22D-03

Cycle 12 Pass 1 IDiag 1:

RMSU= 5.71D-07 CP: 1.00D+00 2.04D+00 2.02D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.64D+00 1.74D+00 1.17D+00

CP: 9.62D-01

E= -1276.01371685036 Delta-E= -0.000000149374 Rises=F Damp=F

DIIS: error= 3.82D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1276.01371685036 IErMin=12 ErrMin= 3.82D-06

ErrMax= 3.82D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.85D-08 BMatP= 1.63D-07

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

Coeff-Com: 0.417D-03-0.642D-02-0.832D-02-0.192D-01-0.145D-01 0.809D-01

Coeff-Com: -0.164D-01-0.287D-01-0.129D+00 0.113D+00 0.371D+00 0.657D+00

Coeff: 0.417D-03-0.642D-02-0.832D-02-0.192D-01-0.145D-01 0.809D-01

Coeff: -0.164D-01-0.287D-01-0.129D+00 0.113D+00 0.371D+00 0.657D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=3.90D-07 MaxDP=1.75D-05 DE=-1.49D-07 OVMax= 2.76D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.34D-07 CP: 1.00D+00 2.04D+00 2.02D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.66D+00 1.76D+00 1.23D+00

CP: 1.03D+00 1.08D+00

E= -1276.01371686172 Delta-E= -0.000000011360 Rises=F Damp=F

DIIS: error= 1.73D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1276.01371686172 IErMin=13 ErrMin= 1.73D-06

ErrMax= 1.73D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.33D-09 BMatP= 1.85D-08

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

Coeff-Com: -0.372D-04 0.168D-02 0.891D-03-0.118D-02-0.675D-02-0.667D-02

Coeff-Com: 0.262D-01 0.714D-02-0.280D-01-0.912D-01-0.467D-01 0.254D+00

Coeff-Com: 0.891D+00

Coeff: -0.372D-04 0.168D-02 0.891D-03-0.118D-02-0.675D-02-0.667D-02

Coeff: 0.262D-01 0.714D-02-0.280D-01-0.912D-01-0.467D-01 0.254D+00

Coeff: 0.891D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=1.91D-07 MaxDP=1.21D-05 DE=-1.14D-08 OVMax= 1.15D-04

Cycle 14 Pass 1 IDiag 1:

RMSU= 7.52D-08 CP: 9.99D-01 2.04D+00 2.03D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.67D+00 1.77D+00 1.25D+00

CP: 1.09D+00 1.16D+00 1.08D+00

E= -1276.01371686488 Delta-E= -0.000000003167 Rises=F Damp=F

DIIS: error= 1.10D-06 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1276.01371686488 IErMin=14 ErrMin= 1.10D-06

ErrMax= 1.10D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.53D-09 BMatP= 3.33D-09

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

Coeff-Com: -0.915D-04 0.223D-02 0.190D-02 0.211D-02-0.254D-02-0.190D-01

Coeff-Com: 0.211D-01 0.935D-02 0.579D-02-0.821D-01-0.988D-01 0.498D-01

Coeff-Com: 0.578D+00 0.533D+00

Coeff: -0.915D-04 0.223D-02 0.190D-02 0.211D-02-0.254D-02-0.190D-01

Coeff: 0.211D-01 0.935D-02 0.579D-02-0.821D-01-0.988D-01 0.498D-01

Coeff: 0.578D+00 0.533D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=1.95D-07 MaxDP=7.53D-06 DE=-3.17D-09 OVMax= 1.50D-04

Cycle 15 Pass 1 IDiag 1:

RMSU= 3.07D-08 CP: 9.99D-01 2.04D+00 2.03D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.68D+00 1.78D+00 1.26D+00

CP: 1.10D+00 1.23D+00 1.25D+00 9.76D-01

E= -1276.01371686596 Delta-E= -0.000000001072 Rises=F Damp=F

DIIS: error= 3.62D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1276.01371686596 IErMin=15 ErrMin= 3.62D-07

ErrMax= 3.62D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.39D-10 BMatP= 1.53D-09

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

Coeff-Com: -0.200D-04 0.137D-03 0.423D-03 0.112D-02 0.161D-02-0.403D-02

Coeff-Com: -0.160D-02-0.507D-03 0.120D-01 0.298D-02-0.186D-01-0.698D-01

Coeff-Com: -0.105D+00 0.169D+00 0.101D+01

Coeff: -0.200D-04 0.137D-03 0.423D-03 0.112D-02 0.161D-02-0.403D-02

Coeff: -0.160D-02-0.507D-03 0.120D-01 0.298D-02-0.186D-01-0.698D-01

Coeff: -0.105D+00 0.169D+00 0.101D+01

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=6.68D-08 MaxDP=3.99D-06 DE=-1.07D-09 OVMax= 4.64D-05

Cycle 16 Pass 1 IDiag 1:

RMSU= 1.23D-08 CP: 9.99D-01 2.04D+00 2.03D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.68D+00 1.79D+00 1.27D+00

CP: 1.11D+00 1.26D+00 1.34D+00 1.21D+00 1.23D+00

E= -1276.01371686612 Delta-E= -0.000000000160 Rises=F Damp=F

DIIS: error= 1.88D-07 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1276.01371686612 IErMin=16 ErrMin= 1.88D-07

ErrMax= 1.88D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.94D-11 BMatP= 1.39D-10

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

Coeff-Com: 0.134D-05-0.211D-03-0.242D-04 0.391D-03 0.123D-02 0.198D-03

Coeff-Com: -0.381D-02-0.127D-02 0.548D-02 0.127D-01 0.393D-02-0.404D-01

Coeff-Com: -0.122D+00 0.824D-02 0.443D+00 0.692D+00

Coeff: 0.134D-05-0.211D-03-0.242D-04 0.391D-03 0.123D-02 0.198D-03

Coeff: -0.381D-02-0.127D-02 0.548D-02 0.127D-01 0.393D-02-0.404D-01

Coeff: -0.122D+00 0.824D-02 0.443D+00 0.692D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=1.39D-08 MaxDP=9.92D-07 DE=-1.60D-10 OVMax= 8.27D-06

Cycle 17 Pass 1 IDiag 1:

RMSU= 5.72D-09 CP: 9.99D-01 2.04D+00 2.03D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.68D+00 1.79D+00 1.27D+00

CP: 1.11D+00 1.26D+00 1.36D+00 1.26D+00 1.37D+00

CP: 1.05D+00

E= -1276.01371686611 Delta-E= 0.000000000010 Rises=F Damp=F

DIIS: error= 1.39D-07 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=16 EnMin= -1276.01371686612 IErMin=17 ErrMin= 1.39D-07

ErrMax= 1.39D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.06D-11 BMatP= 2.94D-11

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

Coeff-Com: 0.502D-05-0.140D-03-0.134D-03-0.791D-04 0.259D-03 0.101D-02

Coeff-Com: -0.144D-02-0.325D-03-0.537D-04 0.575D-02 0.617D-02-0.608D-02

Coeff-Com: -0.399D-01-0.299D-01-0.559D-04 0.380D+00 0.685D+00

Coeff: 0.502D-05-0.140D-03-0.134D-03-0.791D-04 0.259D-03 0.101D-02

Coeff: -0.144D-02-0.325D-03-0.537D-04 0.575D-02 0.617D-02-0.608D-02

Coeff: -0.399D-01-0.299D-01-0.559D-04 0.380D+00 0.685D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.094 Goal= None Shift= 0.000

RMSDP=5.47D-09 MaxDP=3.72D-07 DE= 1.05D-11 OVMax= 2.63D-06

Error on total polarization charges = 0.06995

SCF Done: E(UB3LYP) = -1276.01371687 A.U. after 17 cycles

NFock= 17 Conv=0.55D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7689 S= 0.5094

<L.S>= 0.000000000000E+00

KE= 1.320983228744D+03 PE=-8.596458884491D+03 EE= 3.241048032594D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.67

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7689, after 0.7502

Leave Link 502 at Tue Sep 17 13:56:19 2019, MaxMem= 2415919104 cpu: 1649.0

(Enter /home/blab/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15305 LenP2D= 41192.

LDataN: DoStor=T MaxTD1= 6 Len= 172

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

GePol: Maximum number of non-zero 1st derivatives = 251

Leave Link 701 at Tue Sep 17 13:56:23 2019, MaxMem= 2415919104 cpu: 66.6

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 13:56:23 2019, MaxMem= 2415919104 cpu: 0.3

(Enter /home/blab/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

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

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

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

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

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Tue Sep 17 13:56:36 2019, MaxMem= 2415919104 cpu: 227.8

(Enter /home/blab/g09/l716.exe)

Dipole = 9.94759830D-14-1.23012711D-13-2.22044605D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.011841132 0.003816228 -0.000000000

2 7 -0.008415520 0.005722959 0.000000000

3 6 0.005494152 -0.005484147 0.000000000

4 6 0.000569482 -0.000867897 -0.000000000

5 6 -0.001872742 -0.003060792 -0.000000000

6 7 0.000337185 0.007515554 -0.000000000

7 6 -0.005494502 -0.011867355 0.000000000

8 7 0.004335395 0.008360227 0.000000000

9 6 -0.013003555 0.000392598 0.000000000

10 6 0.005320310 -0.006658192 -0.000000000

11 6 0.001371153 0.003980357 -0.000000000

12 7 -0.006079523 0.000074670 0.000000000

13 6 -0.005320310 0.006658192 -0.000000000

14 6 -0.001371153 -0.003980357 -0.000000000

15 6 0.005494502 0.011867355 0.000000000

16 7 -0.004335395 -0.008360227 0.000000000

17 6 0.013003555 -0.000392598 0.000000000

18 7 -0.000337185 -0.007515554 0.000000000

19 7 0.008415520 -0.005722959 0.000000000

20 6 -0.005494152 0.005484147 0.000000000

21 6 -0.000569482 0.000867897 -0.000000000

22 6 0.001872742 0.003060792 0.000000000

23 6 -0.011841132 -0.003816228 0.000000000

24 7 0.006079523 -0.000074670 -0.000000000

25 30 -0.000000000 0.000000000 -0.000000000

26 6 -0.000589714 -0.000895131 0.000000000

27 1 0.000075315 0.000022477 -0.000000000

28 6 0.000515981 0.000582816 -0.000000000

29 1 -0.000555045 0.000184050 -0.000000000

30 6 -0.000515981 -0.000582816 -0.000000000

31 1 0.000555045 -0.000184050 0.000000000

32 6 0.000589714 0.000895131 0.000000000

33 1 -0.000075315 -0.000022477 -0.000000000

34 1 -0.000388323 0.000463379 0.000000000

35 1 0.000183683 0.000313997 0.001028436

36 1 0.000183683 0.000313997 -0.001028436

37 1 -0.000119138 0.000482784 0.001095116

38 1 -0.000119138 0.000482784 -0.001095116

39 1 -0.000255644 -0.000390009 0.000000000

40 1 0.000119138 -0.000482784 0.001095116

41 1 0.000119138 -0.000482784 -0.001095116

42 1 0.000255644 0.000390009 -0.000000000

43 1 -0.000183683 -0.000313997 0.001028436

44 1 -0.000183683 -0.000313997 -0.001028436

45 1 0.000388323 -0.000463379 -0.000000000

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

Cartesian Forces: Max 0.013003555 RMS 0.003758263

Leave Link 716 at Tue Sep 17 13:56:36 2019, MaxMem= 2415919104 cpu: 0.3

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

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

Internal Forces: Max 0.006653649 RMS 0.001442978

Search for a local minimum.

Step number 4 out of a maximum of 270

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

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4

DE= -1.37D-04 DEPred=-6.56D-04 R= 2.09D-01

Trust test= 2.09D-01 RLast= 1.21D-01 DXMaxT set to 3.00D-01

ITU= 0 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01333

Eigenvalues --- 0.01335 0.01335 0.01336 0.01610 0.01628

Eigenvalues --- 0.01640 0.01645 0.01769 0.01787 0.01805

Eigenvalues --- 0.01809 0.01887 0.01903 0.01938 0.01945

Eigenvalues --- 0.01997 0.01998 0.02043 0.02051 0.02070

Eigenvalues --- 0.02086 0.02101 0.02110 0.02112 0.02205

Eigenvalues --- 0.02312 0.02320 0.02352 0.02374 0.07104

Eigenvalues --- 0.07104 0.07147 0.07147 0.07181 0.07195

Eigenvalues --- 0.07257 0.07275 0.12784 0.14483 0.14506

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 0.16015 0.16065

Eigenvalues --- 0.16388 0.17115 0.19424 0.22073 0.22102

Eigenvalues --- 0.23852 0.23857 0.23868 0.24111 0.24999

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25699

Eigenvalues --- 0.26300 0.32075 0.33209 0.33217 0.33281

Eigenvalues --- 0.33282 0.33282 0.33321 0.33541 0.33724

Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33842 0.34070 0.34437 0.34437

Eigenvalues --- 0.34439 0.34461 0.35534 0.35542 0.35681

Eigenvalues --- 0.35682 0.35682 0.35771 0.36782 0.38552

Eigenvalues --- 0.41615 0.41677 0.41750 0.43146 0.47935

Eigenvalues --- 0.48936 0.49014 0.50267 0.51357 0.51368

Eigenvalues --- 0.51687 0.52133 0.53770 0.53983 0.54054

Eigenvalues --- 0.56308 0.56366 0.56561 1.01316

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 0.50642 0.49358

Cosine: 1.000 > 0.970

Length: 1.000

GDIIS step was calculated using 2 of the last 4 vectors.

Iteration 1 RMS(Cart)= 0.00351848 RMS(Int)= 0.00000661

Iteration 2 RMS(Cart)= 0.00001321 RMS(Int)= 0.00000375

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000375

ITry= 1 IFail=0 DXMaxC= 1.15D-02 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.72D-10 for atom 33.

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

(Linear) (Quad) (Total)

R1 2.62149 -0.00661 -0.00831 -0.00167 -0.00999 2.61150

R2 2.70482 0.00315 0.01265 -0.00098 0.01167 2.71649

R3 2.55629 0.00264 -0.00872 0.00481 -0.00391 2.55238

R4 2.55199 0.00488 0.00541 0.00111 0.00652 2.55851

R5 3.81141 -0.00222 -0.00186 -0.00345 -0.00531 3.80610

R6 2.74127 0.00056 0.01189 -0.00264 0.00925 2.75052

R7 2.59031 -0.00332 -0.01656 0.00394 -0.01262 2.57769

R8 2.61782 0.00000 -0.00861 0.00273 -0.00587 2.61195

R9 2.82332 -0.00037 -0.00054 -0.00037 -0.00091 2.82242

R10 2.04618 -0.00008 -0.00031 0.00011 -0.00020 2.04598

R11 2.53663 -0.00665 0.00455 -0.00600 -0.00144 2.53519

R12 2.55680 0.00434 0.00439 0.00124 0.00563 2.56243

R13 2.77106 0.00121 -0.00669 0.00428 -0.00241 2.76866

R14 2.62396 -0.00601 -0.00964 -0.00089 -0.01052 2.61344

R15 3.80211 -0.00218 0.00147 -0.00498 -0.00351 3.79860

R16 2.76683 0.00556 -0.00228 0.00734 0.00506 2.77189

R17 2.49329 0.00015 0.01243 -0.00434 0.00810 2.50139

R18 2.58080 -0.00225 0.00502 -0.00378 0.00124 2.58203

R19 2.81684 0.00035 0.00154 -0.00051 0.00103 2.81787

R20 2.04563 -0.00044 -0.00008 -0.00017 -0.00025 2.04538

R21 2.49329 0.00015 0.01243 -0.00434 0.00810 2.50139

R22 2.58080 -0.00225 0.00502 -0.00378 0.00124 2.58203

R23 2.76683 0.00556 -0.00228 0.00734 0.00506 2.77189

R24 2.81684 0.00035 0.00154 -0.00051 0.00103 2.81787

R25 2.77106 0.00121 -0.00669 0.00428 -0.00241 2.76866

R26 2.04563 -0.00044 -0.00008 -0.00017 -0.00025 2.04538

R27 2.55680 0.00434 0.00439 0.00124 0.00563 2.56243

R28 2.53663 -0.00665 0.00455 -0.00600 -0.00144 2.53519

R29 2.62396 -0.00601 -0.00964 -0.00089 -0.01052 2.61344

R30 3.80211 -0.00218 0.00147 -0.00498 -0.00351 3.79860

R31 2.59031 -0.00332 -0.01656 0.00394 -0.01262 2.57769

R32 2.55199 0.00488 0.00541 0.00111 0.00652 2.55851

R33 2.62149 -0.00661 -0.00831 -0.00167 -0.00999 2.61150

R34 3.81141 -0.00222 -0.00186 -0.00345 -0.00531 3.80610

R35 2.74127 0.00056 0.01189 -0.00264 0.00925 2.75052

R36 2.61782 0.00000 -0.00861 0.00273 -0.00587 2.61195

R37 2.82332 -0.00037 -0.00054 -0.00037 -0.00091 2.82242

R38 2.70482 0.00315 0.01265 -0.00098 0.01167 2.71649

R39 2.04618 -0.00008 -0.00031 0.00011 -0.00020 2.04598

R40 2.55629 0.00264 -0.00872 0.00481 -0.00391 2.55238

R41 2.06475 0.00002 -0.00036 0.00034 -0.00001 2.06473

R42 2.06819 0.00085 0.00047 0.00111 0.00159 2.06977

R43 2.06819 0.00085 0.00047 0.00111 0.00159 2.06977

R44 2.06606 0.00112 0.00079 0.00131 0.00211 2.06816

R45 2.06606 0.00112 0.00079 0.00131 0.00211 2.06816

R46 2.06256 0.00015 0.00035 0.00018 0.00053 2.06309

R47 2.06606 0.00112 0.00079 0.00131 0.00211 2.06816

R48 2.06606 0.00112 0.00079 0.00131 0.00211 2.06816

R49 2.06256 0.00015 0.00035 0.00018 0.00053 2.06309

R50 2.06819 0.00085 0.00047 0.00111 0.00159 2.06977

R51 2.06819 0.00085 0.00047 0.00111 0.00159 2.06977

R52 2.06475 0.00002 -0.00036 0.00034 -0.00001 2.06473

A1 1.87714 0.00156 0.00110 0.00253 0.00363 1.88078

A2 2.19744 0.00066 0.00680 -0.00248 0.00431 2.20175

A3 2.20860 -0.00222 -0.00790 -0.00005 -0.00794 2.20066

A4 1.90932 -0.00035 0.00214 -0.00337 -0.00124 1.90809

A5 2.17933 0.00066 0.00212 0.00073 0.00285 2.18217

A6 2.19454 -0.00031 -0.00426 0.00264 -0.00161 2.19292

A7 1.89848 -0.00003 -0.00403 0.00359 -0.00046 1.89803

A8 2.22884 -0.00116 0.00156 -0.00347 -0.00190 2.22694

A9 2.15586 0.00119 0.00247 -0.00012 0.00235 2.15821

A10 1.85474 -0.00089 0.00173 -0.00217 -0.00044 1.85430

A11 2.17800 0.00137 -0.00356 0.00386 0.00030 2.17830

A12 2.25044 -0.00048 0.00184 -0.00169 0.00014 2.25059

A13 1.88509 -0.00030 -0.00093 -0.00058 -0.00150 1.88359

A14 2.18294 0.00017 -0.00244 0.00176 -0.00069 2.18225

A15 2.21516 0.00013 0.00337 -0.00118 0.00218 2.21734

A16 2.15234 0.00163 0.00616 -0.00010 0.00606 2.15840

A17 2.22977 0.00067 -0.00271 0.00072 -0.00200 2.22777

A18 2.16310 0.00097 0.00623 -0.00199 0.00425 2.16735

A19 1.89031 -0.00164 -0.00352 0.00127 -0.00225 1.88806

A20 1.90745 0.00110 0.00229 -0.00087 0.00141 1.90886

A21 2.20399 -0.00109 -0.00494 0.00125 -0.00371 2.20027

A22 2.17175 -0.00001 0.00265 -0.00037 0.00230 2.17405

A23 1.88235 0.00035 0.00245 -0.00013 0.00231 1.88467

A24 2.22086 0.00172 0.00154 0.00079 0.00235 2.22320

A25 2.17997 -0.00207 -0.00399 -0.00066 -0.00466 2.17531

A26 1.86535 -0.00081 -0.00394 0.00034 -0.00360 1.86175

A27 2.17760 -0.00104 -0.00024 -0.00098 -0.00122 2.17638

A28 2.24023 0.00185 0.00418 0.00064 0.00482 2.24505

A29 1.87931 0.00100 0.00272 -0.00061 0.00212 1.88143

A30 2.18150 -0.00089 -0.00287 0.00024 -0.00264 2.17886

A31 2.22237 -0.00011 0.00015 0.00037 0.00052 2.22289

A32 2.21229 -0.00277 -0.00892 0.00029 -0.00863 2.20366

A33 1.86535 -0.00081 -0.00394 0.00034 -0.00360 1.86175

A34 2.24023 0.00185 0.00418 0.00064 0.00482 2.24505

A35 2.17760 -0.00104 -0.00024 -0.00098 -0.00122 2.17638

A36 1.87931 0.00100 0.00272 -0.00061 0.00212 1.88143

A37 2.22237 -0.00011 0.00015 0.00037 0.00052 2.22289

A38 2.18150 -0.00089 -0.00287 0.00024 -0.00264 2.17886

A39 1.89031 -0.00164 -0.00352 0.00127 -0.00225 1.88806

A40 2.16310 0.00097 0.00623 -0.00199 0.00425 2.16735

A41 2.22977 0.00067 -0.00271 0.00072 -0.00200 2.22777

A42 1.90745 0.00110 0.00229 -0.00087 0.00141 1.90886

A43 2.20399 -0.00109 -0.00494 0.00125 -0.00371 2.20027

A44 2.17175 -0.00001 0.00265 -0.00037 0.00230 2.17405

A45 2.17997 -0.00207 -0.00399 -0.00066 -0.00466 2.17531

A46 2.22086 0.00172 0.00154 0.00079 0.00235 2.22320

A47 1.88235 0.00035 0.00245 -0.00013 0.00231 1.88467

A48 2.15234 0.00163 0.00616 -0.00010 0.00606 2.15840

A49 1.90932 -0.00035 0.00214 -0.00337 -0.00124 1.90809

A50 2.19454 -0.00031 -0.00426 0.00264 -0.00161 2.19292

A51 2.17933 0.00066 0.00212 0.00073 0.00285 2.18217

A52 2.22884 -0.00116 0.00156 -0.00347 -0.00190 2.22694

A53 2.15586 0.00119 0.00247 -0.00012 0.00235 2.15821

A54 1.89848 -0.00003 -0.00403 0.00359 -0.00046 1.89803

A55 1.85474 -0.00089 0.00173 -0.00217 -0.00044 1.85430

A56 2.17800 0.00137 -0.00356 0.00386 0.00030 2.17830

A57 2.25044 -0.00048 0.00184 -0.00169 0.00014 2.25059

A58 1.88509 -0.00030 -0.00093 -0.00058 -0.00150 1.88359

A59 2.21516 0.00013 0.00337 -0.00118 0.00218 2.21734

A60 2.18294 0.00017 -0.00244 0.00176 -0.00069 2.18225

A61 1.87714 0.00156 0.00110 0.00253 0.00363 1.88078

A62 2.19744 0.00066 0.00680 -0.00248 0.00431 2.20175

A63 2.20860 -0.00222 -0.00790 -0.00005 -0.00794 2.20066

A64 2.21229 -0.00277 -0.00892 0.00029 -0.00863 2.20366

A65 1.55689 0.00026 0.00420 -0.00103 0.00317 1.56006

A66 1.58470 -0.00026 -0.00420 0.00103 -0.00317 1.58154

A67 1.58470 -0.00026 -0.00420 0.00103 -0.00317 1.58154

A68 1.55689 0.00026 0.00420 -0.00103 0.00317 1.56006

A69 1.94947 -0.00067 -0.00214 -0.00096 -0.00310 1.94638

A70 1.95228 -0.00053 -0.00265 -0.00040 -0.00305 1.94923

A71 1.95228 -0.00053 -0.00265 -0.00040 -0.00305 1.94923

A72 1.87809 0.00053 0.00253 0.00010 0.00264 1.88073

A73 1.87809 0.00053 0.00253 0.00010 0.00264 1.88073

A74 1.84840 0.00083 0.00294 0.00171 0.00466 1.85306

A75 1.94411 -0.00037 -0.00029 -0.00091 -0.00120 1.94290

A76 1.94411 -0.00037 -0.00029 -0.00091 -0.00120 1.94290

A77 1.94751 -0.00048 -0.00137 -0.00093 -0.00230 1.94521

A78 1.85277 0.00052 0.00222 0.00105 0.00327 1.85604

A79 1.88570 0.00040 -0.00005 0.00095 0.00090 1.88660

A80 1.88570 0.00040 -0.00005 0.00095 0.00090 1.88660

A81 1.94411 -0.00037 -0.00029 -0.00091 -0.00120 1.94290

A82 1.94411 -0.00037 -0.00029 -0.00091 -0.00120 1.94290

A83 1.94751 -0.00048 -0.00137 -0.00093 -0.00230 1.94521

A84 1.85277 0.00052 0.00222 0.00105 0.00327 1.85604

A85 1.88570 0.00040 -0.00005 0.00095 0.00090 1.88660

A86 1.88570 0.00040 -0.00005 0.00095 0.00090 1.88660

A87 1.95228 -0.00053 -0.00265 -0.00040 -0.00305 1.94923

A88 1.95228 -0.00053 -0.00265 -0.00040 -0.00305 1.94923

A89 1.94947 -0.00067 -0.00214 -0.00096 -0.00310 1.94638

A90 1.84840 0.00083 0.00294 0.00171 0.00466 1.85306

A91 1.87809 0.00053 0.00253 0.00010 0.00264 1.88073

A92 1.87809 0.00053 0.00253 0.00010 0.00264 1.88073

A93 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

A94 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

A95 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

A96 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D1 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D2 3.14159 0.00000 -0.00000 -0.00000 0.00000 3.14159

D3 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D4 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D6 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

D7 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D10 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

D11 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D12 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

D13 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

D14 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D15 3.14159 0.00000 -0.00000 -0.00000 0.00000 3.14159

D16 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D17 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D18 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D19 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D20 3.14159 0.00000 -0.00000 -0.00000 0.00000 3.14159

D21 3.14159 0.00000 -0.00000 -0.00000 0.00000 3.14159

D22 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D23 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D24 3.14159 0.00000 -0.00000 -0.00000 0.00000 3.14159

D25 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D26 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

D27 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D28 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D29 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

D30 1.03519 0.00017 0.00009 0.00082 0.00091 1.03610

D31 -1.03519 -0.00017 -0.00009 -0.00082 -0.00091 -1.03610

D32 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.10640 0.00017 0.00009 0.00082 0.00091 -2.10550

D34 2.10640 -0.00017 -0.00009 -0.00082 -0.00091 2.10550

D35 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D36 3.14159 0.00000 -0.00000 -0.00000 0.00000 3.14159

D37 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

D38 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D39 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D40 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

D41 3.14159 0.00000 -0.00000 -0.00000 0.00000 3.14159

D42 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D43 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D44 3.14159 0.00000 -0.00000 -0.00000 0.00000 3.14159

D45 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D46 3.14159 0.00000 -0.00000 -0.00000 0.00000 3.14159

D47 3.14159 0.00000 -0.00000 -0.00000 0.00000 3.14159

D48 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D49 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D50 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

D51 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D52 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D53 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D54 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

D55 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D56 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D57 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D58 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D59 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D60 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D61 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

D62 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D63 1.03251 0.00008 0.00120 0.00006 0.00127 1.03378

D64 -1.03251 -0.00008 -0.00120 -0.00006 -0.00127 -1.03378

D65 3.14159 0.00000 -0.00000 -0.00000 0.00000 3.14159

D66 -2.10908 0.00008 0.00120 0.00006 0.00127 -2.10782

D67 2.10908 -0.00008 -0.00120 -0.00006 -0.00127 2.10782

D68 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D69 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D70 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D71 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D72 3.14159 0.00000 -0.00000 -0.00000 0.00000 3.14159

D73 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D74 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D75 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

D76 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D77 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D78 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D79 -2.10908 0.00008 0.00120 0.00006 0.00127 -2.10782

D80 2.10908 -0.00008 -0.00120 -0.00006 -0.00127 2.10782

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 1.03251 0.00008 0.00120 0.00006 0.00127 1.03378

D83 -1.03251 -0.00008 -0.00120 -0.00006 -0.00127 -1.03378

D84 3.14159 0.00000 -0.00000 -0.00000 0.00000 3.14159

D85 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D86 3.14159 0.00000 -0.00000 -0.00000 0.00000 3.14159

D87 3.14159 0.00000 -0.00000 -0.00000 0.00000 3.14159

D88 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D89 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D90 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

D91 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

D92 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D93 3.14159 0.00000 -0.00000 -0.00000 0.00000 3.14159

D94 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D95 3.14159 0.00000 -0.00000 -0.00000 0.00000 3.14159

D96 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D97 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D98 3.14159 0.00000 -0.00000 -0.00000 0.00000 3.14159

D99 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

D100 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D101 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D102 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D103 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D104 3.14159 0.00000 -0.00000 -0.00000 0.00000 3.14159

D105 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

D106 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D107 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D108 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

D109 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D110 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D111 3.14159 0.00000 -0.00000 -0.00000 0.00000 3.14159

D112 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D113 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D114 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D116 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D117 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D118 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D119 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D120 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D121 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D122 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D123 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D124 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D125 1.03519 0.00017 0.00009 0.00082 0.00091 1.03610

D126 -1.03519 -0.00017 -0.00009 -0.00082 -0.00091 -1.03610

D127 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

D128 -2.10640 0.00017 0.00009 0.00082 0.00091 -2.10550

D129 2.10640 -0.00017 -0.00009 -0.00082 -0.00091 2.10550

D130 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D131 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D132 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D133 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

D134 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D135 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D136 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

Item Value Threshold Converged?

Maximum Force 0.006654 0.000450 NO

RMS Force 0.001443 0.000300 NO

Maximum Displacement 0.011487 0.001800 NO

RMS Displacement 0.003524 0.001200 NO

Predicted change in Energy=-4.523087D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 13:56:36 2019, MaxMem= 2415919104 cpu: 1.7

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.081968 -2.197059 -0.000000

2 7 0 -0.738342 -1.873887 -0.000000

3 6 0 -0.003938 -3.011300 -0.000000

4 6 0 -0.908059 -4.151950 -0.000000

5 6 0 -2.188162 -3.630637 -0.000000

6 7 0 1.355443 -3.124138 -0.000000

7 6 0 2.188974 -2.072941 -0.000000

8 7 0 1.862175 -0.756929 -0.000000

9 6 0 3.017869 0.002667 -0.000000

10 6 0 4.162605 -0.914471 -0.000000

11 6 0 3.650089 -2.181061 -0.000000

12 7 0 -3.111696 -1.323016 -0.000000

13 6 0 -4.162605 0.914471 -0.000000

14 6 0 -3.650089 2.181061 -0.000000

15 6 0 -2.188974 2.072941 -0.000000

16 7 0 -1.862175 0.756929 -0.000000

17 6 0 -3.017869 -0.002667 -0.000000

18 7 0 -1.355443 3.124138 -0.000000

19 7 0 0.738342 1.873887 -0.000000

20 6 0 0.003938 3.011300 -0.000000

21 6 0 0.908059 4.151950 -0.000000

22 6 0 2.188162 3.630637 -0.000000

23 6 0 2.081968 2.197059 -0.000000

24 7 0 3.111696 1.323016 -0.000000

25 30 0 0.000000 -0.000000 -0.000000

26 6 0 -0.476601 -5.581831 -0.000000

27 1 0 -3.118171 -4.184976 -0.000000

28 6 0 5.591598 -0.488422 -0.000000

29 1 0 4.201182 -3.112629 -0.000000

30 6 0 -5.591598 0.488422 -0.000000

31 1 0 -4.201182 3.112629 -0.000000

32 6 0 0.476601 5.581831 -0.000000

33 1 0 3.118171 4.184976 -0.000000

34 1 0 -1.333937 -6.259160 -0.000000

35 1 0 0.136831 -5.819424 0.875718

36 1 0 0.136831 -5.819424 -0.875718

37 1 0 5.823898 0.125091 0.876015

38 1 0 5.823898 0.125091 -0.876015

39 1 0 6.264550 -1.348091 -0.000000

40 1 0 -5.823898 -0.125091 0.876015

41 1 0 -5.823898 -0.125091 -0.876015

42 1 0 -6.264550 1.348091 -0.000000

43 1 0 -0.136831 5.819424 0.875718

44 1 0 -0.136831 5.819424 -0.875718

45 1 0 1.333937 6.259160 -0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.381945 0.000000

3 C 2.231860 1.353905 0.000000

4 C 2.280277 2.284376 1.455512 0.000000

5 C 1.437506 2.277751 2.270333 1.382184 0.000000

6 N 3.560235 2.438660 1.364056 2.485928 3.579620

7 C 4.272745 2.934076 2.385243 3.730133 4.646046

8 N 4.198838 2.830244 2.926528 4.381822 4.966229

9 C 5.554019 4.198878 4.267941 5.716096 6.348516

10 C 6.374929 4.993972 4.664416 6.016054 6.907228

11 C 5.732079 4.399168 3.747160 4.965996 6.015517

12 N 1.350663 2.436446 3.536731 3.585929 2.485564

13 C 3.743083 4.415939 5.718933 6.021685 4.955444

14 C 4.650477 4.992081 6.344685 6.901142 5.992751

15 C 4.271340 4.204971 5.533886 6.355313 5.703577

16 N 2.962154 2.860803 4.201500 5.000743 4.399659

17 C 2.385638 2.949188 4.258598 4.654874 3.721637

18 N 5.370566 5.035978 6.282529 7.289829 6.805910

19 N 4.952449 4.028201 4.941259 6.246707 6.234116

20 C 5.610527 4.941259 6.022606 7.221073 6.994329

21 C 7.017847 6.246707 7.221073 8.500179 8.375872

22 C 7.224683 6.234116 6.994329 8.375872 8.478108

23 C 6.053646 4.952449 5.610527 7.017847 7.224683

24 N 6.274160 5.004297 5.337928 6.792178 7.254459

25 Zn 3.026823 2.014101 3.011303 4.250089 4.239054

26 C 3.746183 3.717171 2.613626 1.493558 2.595496

27 H 2.241769 3.317336 3.328056 2.210359 1.082685

28 C 7.861492 6.479787 6.137991 7.461030 8.390362

29 H 6.349507 5.092482 4.206341 5.213879 6.410309

30 C 4.419198 5.397647 6.593178 6.593071 5.343222

31 H 5.716979 6.070964 7.424242 7.976137 7.037320

32 C 8.188859 7.554060 8.606557 9.831774 9.590127

33 H 8.232364 7.182096 7.844358 9.258232 9.446744

34 H 4.130401 4.425534 3.509628 2.149815 2.763844

35 H 4.337221 4.135223 2.944870 2.153868 3.311082

36 H 4.337221 4.135223 2.944870 2.153868 3.311082

37 H 8.286284 6.915657 6.675929 8.023698 8.891907

38 H 8.286284 6.915657 6.675929 8.023698 8.891907

39 H 8.389583 7.022603 6.485384 7.701165 8.755476

40 H 4.366062 5.448722 6.555116 6.414707 5.125898

41 H 4.366062 5.448722 6.555116 6.414707 5.125898

42 H 5.482890 6.396884 7.628863 7.677398 6.434646

43 H 8.295447 7.766320 8.875035 10.039421 9.709711

44 H 8.295447 7.766320 8.875035 10.039421 9.709711

45 H 9.120090 8.392901 9.366501 10.649777 10.498250

6 7 8 9 10

6 N 0.000000

7 C 1.341563 0.000000

8 N 2.420838 1.355981 0.000000

9 C 3.541267 2.234998 1.382973 0.000000

10 C 3.572505 2.288509 2.305818 1.466821 0.000000

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12 N 4.816573 5.353456 5.005982 6.271284 7.285765

13 C 6.838071 7.019059 6.252324 7.238135 8.523741

14 C 7.293866 7.224347 6.246346 7.014775 8.403601

15 C 6.290669 6.029491 4.941657 5.603325 7.019059

16 N 5.041404 4.941657 4.020268 4.937990 6.252324

17 C 5.373029 5.603325 4.937990 6.035740 7.238135

18 N 6.811010 6.290669 5.041404 5.373029 6.838071

19 N 5.035978 4.204971 2.860803 2.949188 4.415939

20 C 6.282529 5.533886 4.201500 4.258598 5.718933

21 C 7.289829 6.355313 5.000743 4.654874 6.021685

22 C 6.805910 5.703577 4.399659 3.721637 4.955444

23 C 5.370566 4.271340 2.962154 2.385638 3.743083

24 N 4.781382 3.519082 2.426412 1.323679 2.471995

25 Zn 3.405505 3.014745 2.010134 3.017870 4.261870

26 C 3.065394 4.406541 5.361861 6.587711 6.580766

27 H 4.597673 5.711959 6.046102 7.428818 7.981597

28 C 4.989189 3.753471 3.739076 2.620162 1.491153

29 H 2.845763 2.264936 3.319680 3.332461 2.198496

30 C 7.830196 8.191329 7.557091 8.623159 9.854571

31 H 8.353044 8.229473 7.192898 7.860443 9.282805

32 C 8.750215 7.843963 6.488428 6.130670 7.469174

33 H 7.518667 6.326526 5.099015 4.183512 5.205305

34 H 4.130511 5.471319 6.363150 7.625529 7.666660

35 H 3.084876 4.360540 5.419645 6.554693 6.405646

36 H 3.084876 4.360540 5.419645 6.554693 6.405646

37 H 5.593925 4.337214 4.152182 2.942141 2.146623

38 H 5.593925 4.337214 4.152182 2.942141 2.146623

39 H 5.220506 4.139532 4.441889 3.516459 2.146206

40 H 7.829727 8.292626 7.761594 8.885976 10.055882

41 H 7.829727 8.292626 7.761594 8.885976 10.055882

42 H 8.835447 9.119513 8.394925 9.379417 10.669805

43 H 9.109395 8.274399 6.929021 6.674854 8.037249

44 H 9.109395 8.274399 6.929021 6.674854 8.037249

45 H 9.383323 8.375858 7.035946 6.479146 7.711183

11 12 13 14 15

11 C 0.000000

12 N 6.816009 0.000000

13 C 8.403601 2.471995 0.000000

14 C 8.504158 3.545197 1.366354 0.000000

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16 N 6.246346 2.426412 2.305818 2.285779 1.355981

17 C 7.014775 1.323679 1.466821 2.273405 2.234998

18 N 7.293866 4.781382 3.572505 2.480886 1.341563

19 N 4.992081 5.004297 4.993972 4.399168 2.934076

20 C 6.344685 5.337928 4.664416 3.747160 2.385243

21 C 6.901142 6.792178 6.016054 4.965996 3.730133

22 C 5.992751 7.254459 6.907228 6.015517 4.646046

23 C 4.650477 6.274160 6.374929 5.732079 4.272745

24 N 3.545197 6.762552 7.285765 6.816009 5.353456

25 Zn 4.252079 3.381276 4.261870 4.252079 3.014745

26 C 5.347411 5.008116 7.469174 8.386508 7.843963

27 H 7.058683 2.861967 5.205305 6.388221 6.326526

28 C 2.575749 8.743219 9.854571 9.619507 8.191329

29 H 1.082369 7.528672 9.282805 9.469193 8.229473

30 C 9.619507 3.071029 1.491153 2.575749 3.753471

31 H 9.469193 4.567486 2.198496 1.082369 2.264936

32 C 8.386508 7.781568 6.580766 5.347411 4.406541

33 H 6.388221 8.315601 7.981597 7.058683 5.711959

34 H 6.439829 5.246517 7.711183 8.752251 8.375858

35 H 5.132986 5.615825 8.037249 8.894684 8.274399

36 H 5.132986 5.615825 8.037249 8.894684 8.274399

37 H 3.288038 9.094464 10.055882 9.734005 8.292626

38 H 3.288038 9.094464 10.055882 9.734005 8.292626

39 H 2.743947 9.376280 10.669805 10.524019 9.119513

40 H 9.734005 3.091677 2.146623 3.288038 4.337214

41 H 9.734005 3.091677 2.146623 3.288038 4.337214

42 H 10.524019 4.132227 2.146206 2.743947 4.139532

43 H 8.894684 7.786601 6.405646 5.132986 4.360540

44 H 8.894684 7.786601 6.405646 5.132986 4.360540

45 H 8.752251 8.789371 7.666660 6.439829 5.471319

16 17 18 19 20

16 N 0.000000

17 C 1.382973 0.000000

18 N 2.420838 3.541267 0.000000

19 N 2.830244 4.198878 2.438660 0.000000

20 C 2.926528 4.267941 1.364056 1.353905 0.000000

21 C 4.381822 5.716096 2.485928 2.284376 1.455512

22 C 4.966229 6.348516 3.579620 2.277751 2.270333

23 C 4.198838 5.554019 3.560235 1.381945 2.231860

24 N 5.005982 6.271284 4.816573 2.436446 3.536731

25 Zn 2.010134 3.017870 3.405505 2.014101 3.011303

26 C 6.488428 6.130670 8.750215 7.554060 8.606557

27 H 5.099015 4.183512 7.518667 7.182096 7.844358

28 C 7.557091 8.623159 7.830196 5.397647 6.593178

29 H 7.192898 7.860443 8.353044 6.070964 7.424242

30 C 3.739076 2.620162 4.989189 6.479787 6.137991

31 H 3.319680 3.332461 2.845763 5.092482 4.206341

32 C 5.361861 6.587711 3.065394 3.717171 2.613626

33 H 6.046102 7.428818 4.597673 3.317336 3.328056

34 H 7.035946 6.479146 9.383323 8.392901 9.366501

35 H 6.929021 6.674854 9.109395 7.766320 8.875035

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37 H 7.761594 8.885976 7.829727 5.448722 6.555116

38 H 7.761594 8.885976 7.829727 5.448722 6.555116

39 H 8.394925 9.379417 8.835447 6.396884 7.628863

40 H 4.152182 2.942141 5.593925 6.915657 6.675929

41 H 4.152182 2.942141 5.593925 6.915657 6.675929

42 H 4.441889 3.516459 5.220506 7.022603 6.485384

43 H 5.419645 6.554693 3.084876 4.135223 2.944870

44 H 5.419645 6.554693 3.084876 4.135223 2.944870

45 H 6.363150 7.625529 4.130511 4.425534 3.509628

21 22 23 24 25

21 C 0.000000

22 C 1.382184 0.000000

23 C 2.280277 1.437506 0.000000

24 N 3.585929 2.485564 1.350663 0.000000

25 Zn 4.250089 4.239054 3.026823 3.381276 0.000000

26 C 9.831774 9.590127 8.188859 7.781568 5.602141

27 H 9.258232 9.446744 8.232364 8.315601 5.218909

28 C 6.593071 5.343222 4.419198 3.071029 5.612889

29 H 7.976137 7.037320 5.716979 4.567486 5.228613

30 C 7.461030 8.390362 7.861492 8.743219 5.612889

31 H 5.213879 6.410309 6.349507 7.528672 5.228613

32 C 1.493558 2.595496 3.746183 5.008116 5.602141

33 H 2.210359 1.082685 2.241769 2.861967 5.218909

34 H 10.649777 10.498250 9.120090 8.789371 6.399724

35 H 10.039421 9.709711 8.295447 7.786601 5.886536

36 H 10.039421 9.709711 8.295447 7.786601 5.886536

37 H 6.414707 5.125898 4.366062 3.091677 5.890742

38 H 6.414707 5.125898 4.366062 3.091677 5.890742

39 H 7.677398 6.434646 5.482890 4.132227 6.407959

40 H 8.023698 8.891907 8.286284 9.094464 5.890742

41 H 8.023698 8.891907 8.286284 9.094464 5.890742

42 H 7.701165 8.755476 8.389583 9.376280 6.407959

43 H 2.153868 3.311082 4.337221 5.615825 5.886536

44 H 2.153868 3.311082 4.337221 5.615825 5.886536

45 H 2.149815 2.763844 4.130401 5.246517 6.399724

26 27 28 29 30

26 C 0.000000

27 H 2.988159 0.000000

28 C 7.922490 9.461743 0.000000

29 H 5.289482 7.397490 2.969800 0.000000

30 C 7.937957 5.287579 11.225777 10.433892 0.000000

31 H 9.458654 7.377530 10.433892 10.457225 2.969800

32 C 11.204283 10.407349 7.937957 9.458654 7.922490

33 H 10.407349 10.437818 5.287579 7.377530 9.461743

34 H 1.092611 2.736006 9.014679 6.366961 7.978568

35 H 1.095277 3.746110 7.677300 4.961106 8.565670

36 H 1.095277 3.746110 7.677300 4.961106 8.565670

37 H 8.545915 9.965173 1.094425 3.726049 11.454822

38 H 8.545915 9.965173 1.094425 3.726049 11.454822

39 H 7.960382 9.802212 1.091740 2.714973 11.997542

40 H 7.690058 4.956917 11.454822 10.497382 1.094425

41 H 7.690058 4.956917 11.454822 10.497382 1.094425

42 H 9.029074 6.365103 11.997542 11.376712 1.091740

43 H 11.439884 10.475843 8.565670 9.968290 7.677300

44 H 11.439884 10.475843 8.565670 9.968290 7.677300

45 H 11.978611 11.353468 7.978568 9.800588 9.014679

31 32 33 34 35

31 H 0.000000

32 C 5.289482 0.000000

33 H 7.397490 2.988159 0.000000

34 H 9.800588 11.978611 11.353468 0.000000

35 H 9.968290 11.439884 10.475843 1.767316 0.000000

36 H 9.968290 11.439884 10.475843 1.767316 1.751436

37 H 10.497382 7.690058 4.956917 9.631234 8.226785

38 H 10.497382 7.690058 4.956917 9.631234 8.411217

39 H 11.376712 9.029074 6.365103 9.047408 7.636009

40 H 3.726049 8.545915 9.965173 7.652056 8.243526

41 H 3.726049 8.545915 9.965173 7.652056 8.427591

42 H 2.714973 7.960382 9.802212 9.065385 9.649758

43 H 4.961106 1.095277 3.746110 12.169311 11.642065

44 H 4.961106 1.095277 3.746110 12.169311 11.773071

45 H 6.366961 1.092611 2.736006 12.799448 12.169311

36 37 38 39 40

36 H 0.000000

37 H 8.411217 0.000000

38 H 8.226785 1.752031 0.000000

39 H 7.636009 1.769701 1.769701 0.000000

40 H 8.427591 11.650483 11.781484 12.181696 0.000000

41 H 8.243526 11.781484 11.650483 12.181696 1.752031

42 H 9.649758 12.181696 12.181696 12.815918 1.769701

43 H 11.773071 8.243526 8.427591 9.649758 8.226785

44 H 11.642065 8.427591 8.243526 9.649758 8.411217

45 H 12.169311 7.652056 7.652056 9.065385 9.631234

41 42 43 44 45

41 H 0.000000

42 H 1.769701 0.000000

43 H 8.411217 7.636009 0.000000

44 H 8.226785 7.636009 1.751436 0.000000

45 H 9.631234 9.047408 1.767316 1.767316 0.000000

Stoichiometry C20H16N8Zn(1-,2)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=3 Diff= 2.80D-04

Largest Abelian subgroup C2H NOp 4

Largest concise Abelian subgroup C2H NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.953934 0.660253 0.000000

2 7 0 -1.987316 -0.327381 0.000000

3 6 0 -2.586994 -1.541236 0.000000

4 6 0 -4.029915 -1.350201 0.000000

5 6 0 -4.239023 0.016074 0.000000

6 7 0 -1.986576 -2.766041 0.000000

7 6 0 -0.656651 -2.942363 0.000000

8 7 0 0.305417 -1.986796 0.000000

9 6 0 1.550275 -2.589245 0.000000

10 6 0 1.350162 -4.042351 0.000000

11 6 0 0.000000 -4.252079 0.000000

12 7 0 -2.731823 1.992528 0.000000

13 6 0 -1.350162 4.042351 0.000000

14 6 0 0.000000 4.252079 0.000000

15 6 0 0.656651 2.942363 0.000000

16 7 0 -0.305417 1.986796 0.000000

17 6 0 -1.550275 2.589245 0.000000

18 7 0 1.986576 2.766041 0.000000

19 7 0 1.987316 0.327381 0.000000

20 6 0 2.586994 1.541236 0.000000

21 6 0 4.029915 1.350201 0.000000

22 6 0 4.239023 -0.016074 0.000000

23 6 0 2.953934 -0.660253 0.000000

24 7 0 2.731823 -1.992528 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -5.036049 -2.454018 0.000000

27 1 0 -5.191920 0.530073 0.000000

28 6 0 2.448880 -5.050496 0.000000

29 1 0 -0.517003 -5.202989 0.000000

30 6 0 -2.448880 5.050496 0.000000

31 1 0 0.517003 5.202989 0.000000

32 6 0 5.036049 2.454018 0.000000

33 1 0 5.191920 -0.530073 0.000000

34 1 0 -6.057246 -2.065489 0.000000

35 1 0 -4.925350 -3.102474 0.875718

36 1 0 -4.925350 -3.102474 -0.875718

37 1 0 3.094692 -4.935213 0.876015

38 1 0 3.094692 -4.935213 -0.876015

39 1 0 2.056104 -6.069133 0.000000

40 1 0 -3.094692 4.935213 0.876015

41 1 0 -3.094692 4.935213 -0.876015

42 1 0 -2.056104 6.069133 0.000000

43 1 0 4.925350 3.102474 0.875718

44 1 0 4.925350 3.102474 -0.875718

45 1 0 6.057246 2.065489 0.000000

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

Rotational constants (GHZ): 0.1825716 0.1816000 0.0912456

Leave Link 202 at Tue Sep 17 13:56:36 2019, MaxMem= 2415919104 cpu: 0.2

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 229 symmetry adapted cartesian basis functions of AG symmetry.

There are 82 symmetry adapted cartesian basis functions of BG symmetry.

There are 78 symmetry adapted cartesian basis functions of AU symmetry.

There are 218 symmetry adapted cartesian basis functions of BU symmetry.

There are 212 symmetry adapted basis functions of AG symmetry.

There are 82 symmetry adapted basis functions of BG symmetry.

There are 78 symmetry adapted basis functions of AU symmetry.

There are 204 symmetry adapted basis functions of BU symmetry.

576 basis functions, 1015 primitive gaussians, 607 cartesian basis functions

103 alpha electrons 102 beta electrons

nuclear repulsion energy 2759.2942290429 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= 45 NActive= 45 NUniq= 21 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1141257337 Hartrees.

Nuclear repulsion after empirical dispersion term = 2759.1801033091 Hartrees.

No density basis found on file 724.

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

Polarizable Continuum Model (PCM)

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

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

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 = 45

GePol: Total number of spheres = 45

GePol: Number of exposed spheres = 45 (100.00%)

GePol: Number of points = 3606

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.34D-07

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 254

GePol: Fraction of low-weight points (<1% of avg) = 7.04%

GePol: Cavity surface area = 378.926 Ang\*\*2

GePol: Cavity volume = 378.238 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0106466938 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2759.1694566153 Hartrees.

Leave Link 301 at Tue Sep 17 13:56:36 2019, MaxMem= 2415919104 cpu: 2.0

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15309 LenP2D= 41206.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.79D-04 NBF= 212 82 78 204

NBsUse= 576 1.00D-06 EigRej= -1.00D+00 NBFU= 212 82 78 204

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= 594 594 594 594 594 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Tue Sep 17 13:56:37 2019, MaxMem= 2415919104 cpu: 12.1

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 13:56:37 2019, MaxMem= 2415919104 cpu: 1.6

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

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

B after Tr= 0.000000 0.000000 -0.000000

Rot= 1.000000 -0.000000 0.000000 -0.000122 Ang= -0.01 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-BG.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7689 S= 0.5094

Leave Link 401 at Tue Sep 17 13:56:38 2019, MaxMem= 2415919104 cpu: 21.0

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1141655 IEndB= 1141655 NGot= 2415919104 MDV= 2415163146

LenX= 2415163146 LenY= 2414794090

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= 670000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 39009708.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.55D-15 for 3586.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.40D-15 for 1539 694.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.77D-15 for 3586.

Iteration 1 A^-1\*A deviation from orthogonality is 1.83D-11 for 1735 1729.

E= -1276.01401367128

DIIS: error= 4.64D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1276.01401367128 IErMin= 1 ErrMin= 4.64D-04

ErrMax= 4.64D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.43D-04 BMatP= 8.43D-04

IDIUse=3 WtCom= 9.95D-01 WtEn= 4.64D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.291 Goal= None Shift= 0.000

Gap= 0.342 Goal= None Shift= 0.000

RMSDP=4.12D-05 MaxDP=1.17D-03 OVMax= 6.81D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.12D-05 CP: 1.00D+00

E= -1276.01427795735 Delta-E= -0.000264286070 Rises=F Damp=F

DIIS: error= 3.55D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1276.01427795735 IErMin= 2 ErrMin= 3.55D-04

ErrMax= 3.55D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.30D-04 BMatP= 8.43D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.55D-03

Coeff-Com: 0.164D+00 0.836D+00

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

Coeff: 0.163D+00 0.837D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.92D-05 MaxDP=1.13D-03 DE=-2.64D-04 OVMax= 5.46D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.91D-05 CP: 1.00D+00 9.58D-01

E= -1276.01425445051 Delta-E= 0.000023506842 Rises=F Damp=F

DIIS: error= 6.09D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1276.01427795735 IErMin= 2 ErrMin= 3.55D-04

ErrMax= 6.09D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.32D-04 BMatP= 1.30D-04

IDIUse=3 WtCom= 2.88D-01 WtEn= 7.12D-01

Coeff-Com: -0.118D-01 0.580D+00 0.432D+00

Coeff-En: 0.000D+00 0.622D+00 0.378D+00

Coeff: -0.342D-02 0.610D+00 0.394D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.26D-05 MaxDP=5.74D-04 DE= 2.35D-05 OVMax= 3.23D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 3.98D-06 CP: 1.00D+00 1.03D+00 3.92D-01

E= -1276.01430638995 Delta-E= -0.000051939439 Rises=F Damp=F

DIIS: error= 3.89D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1276.01430638995 IErMin= 4 ErrMin= 3.89D-05

ErrMax= 3.89D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.86D-06 BMatP= 1.30D-04

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

Coeff-Com: -0.114D-01 0.210D+00 0.139D+00 0.662D+00

Coeff: -0.114D-01 0.210D+00 0.139D+00 0.662D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.98D-06 MaxDP=9.74D-05 DE=-5.19D-05 OVMax= 3.64D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.75D-06 CP: 1.00D+00 1.03D+00 4.11D-01 7.91D-01

E= -1276.01430681213 Delta-E= -0.000000422184 Rises=F Damp=F

DIIS: error= 3.31D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1276.01430681213 IErMin= 5 ErrMin= 3.31D-05

ErrMax= 3.31D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.28D-06 BMatP= 2.86D-06

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

Coeff-Com: -0.501D-02 0.624D-01 0.367D-01 0.412D+00 0.494D+00

Coeff: -0.501D-02 0.624D-01 0.367D-01 0.412D+00 0.494D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=9.43D-07 MaxDP=4.64D-05 DE=-4.22D-07 OVMax= 1.76D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 5.99D-07 CP: 1.00D+00 1.04D+00 4.04D-01 9.14D-01 7.06D-01

E= -1276.01430712652 Delta-E= -0.000000314392 Rises=F Damp=F

DIIS: error= 7.84D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1276.01430712652 IErMin= 6 ErrMin= 7.84D-06

ErrMax= 7.84D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.16D-08 BMatP= 1.28D-06

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

Coeff-Com: -0.551D-03-0.109D-02-0.181D-02 0.784D-01 0.176D+00 0.749D+00

Coeff: -0.551D-03-0.109D-02-0.181D-02 0.784D-01 0.176D+00 0.749D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=3.76D-07 MaxDP=2.68D-05 DE=-3.14D-07 OVMax= 1.53D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.99D-07 CP: 1.00D+00 1.04D+00 4.09D-01 9.40D-01 8.08D-01

CP: 1.05D+00

E= -1276.01430715734 Delta-E= -0.000000030821 Rises=F Damp=F

DIIS: error= 5.12D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1276.01430715734 IErMin= 7 ErrMin= 5.12D-06

ErrMax= 5.12D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.36D-08 BMatP= 5.16D-08

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

Coeff-Com: 0.109D-02-0.193D-01-0.126D-01-0.711D-01-0.360D-01 0.436D+00

Coeff-Com: 0.702D+00

Coeff: 0.109D-02-0.193D-01-0.126D-01-0.711D-01-0.360D-01 0.436D+00

Coeff: 0.702D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=2.84D-07 MaxDP=1.90D-05 DE=-3.08D-08 OVMax= 1.35D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.69D-07 CP: 1.00D+00 1.04D+00 4.13D-01 9.63D-01 8.46D-01

CP: 1.31D+00 1.34D+00

E= -1276.01430717468 Delta-E= -0.000000017335 Rises=F Damp=F

DIIS: error= 2.66D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1276.01430717468 IErMin= 8 ErrMin= 2.66D-06

ErrMax= 2.66D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.85D-09 BMatP= 2.36D-08

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

Coeff-Com: 0.451D-03-0.377D-02-0.358D-02-0.419D-01-0.667D-01-0.115D+00

Coeff-Com: 0.195D+00 0.104D+01

Coeff: 0.451D-03-0.377D-02-0.358D-02-0.419D-01-0.667D-01-0.115D+00

Coeff: 0.195D+00 0.104D+01

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=3.03D-07 MaxDP=1.55D-05 DE=-1.73D-08 OVMax= 1.98D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.25D-07 CP: 1.00D+00 1.04D+00 4.16D-01 9.82D-01 8.76D-01

CP: 1.51D+00 2.00D+00 1.61D+00

E= -1276.01430718280 Delta-E= -0.000000008124 Rises=F Damp=F

DIIS: error= 1.99D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1276.01430718280 IErMin= 9 ErrMin= 1.99D-06

ErrMax= 1.99D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.04D-09 BMatP= 4.85D-09

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

Coeff-Com: -0.281D-04 0.358D-02 0.101D-02-0.585D-02-0.316D-01-0.193D+00

Coeff-Com: -0.853D-01 0.686D+00 0.626D+00

Coeff: -0.281D-04 0.358D-02 0.101D-02-0.585D-02-0.316D-01-0.193D+00

Coeff: -0.853D-01 0.686D+00 0.626D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.79D-07 MaxDP=8.63D-06 DE=-8.12D-09 OVMax= 1.30D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 6.34D-08 CP: 1.00D+00 1.04D+00 4.18D-01 9.89D-01 8.89D-01

CP: 1.60D+00 2.35D+00 2.15D+00 1.45D+00

E= -1276.01430718583 Delta-E= -0.000000003023 Rises=F Damp=F

DIIS: error= 1.89D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1276.01430718583 IErMin=10 ErrMin= 1.89D-06

ErrMax= 1.89D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.88D-10 BMatP= 3.04D-09

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

Coeff-Com: -0.124D-03 0.296D-02 0.922D-03 0.717D-02 0.168D-03-0.704D-01

Coeff-Com: -0.112D+00 0.118D+00 0.309D+00 0.745D+00

Coeff: -0.124D-03 0.296D-02 0.922D-03 0.717D-02 0.168D-03-0.704D-01

Coeff: -0.112D+00 0.118D+00 0.309D+00 0.745D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.46D-07 MaxDP=5.74D-06 DE=-3.02D-09 OVMax= 1.15D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 2.85D-08 CP: 1.00D+00 1.04D+00 4.20D-01 9.94D-01 8.93D-01

CP: 1.65D+00 2.61D+00 2.54D+00 2.08D+00 1.55D+00

E= -1276.01430718744 Delta-E= -0.000000001613 Rises=F Damp=F

DIIS: error= 1.56D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1276.01430718744 IErMin=11 ErrMin= 1.56D-06

ErrMax= 1.56D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.16D-10 BMatP= 7.88D-10

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

Coeff-Com: -0.286D-04 0.956D-04-0.652D-03 0.462D-02 0.992D-02 0.379D-01

Coeff-Com: -0.308D-01-0.141D+00-0.111D+00 0.214D+00 0.102D+01

Coeff: -0.286D-04 0.956D-04-0.652D-03 0.462D-02 0.992D-02 0.379D-01

Coeff: -0.308D-01-0.141D+00-0.111D+00 0.214D+00 0.102D+01

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.61D-07 MaxDP=6.74D-06 DE=-1.61D-09 OVMax= 1.28D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.92D-08 CP: 1.00D+00 1.04D+00 4.21D-01 9.99D-01 8.95D-01

CP: 1.70D+00 2.87D+00 2.95D+00 2.79D+00 2.45D+00

CP: 1.93D+00

E= -1276.01430718881 Delta-E= -0.000000001370 Rises=F Damp=F

DIIS: error= 1.19D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1276.01430718881 IErMin=12 ErrMin= 1.19D-06

ErrMax= 1.19D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.12D-10 BMatP= 4.16D-10

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

Coeff-Com: 0.896D-04-0.222D-02-0.189D-02-0.425D-02 0.211D-02 0.710D-01

Coeff-Com: 0.537D-01-0.108D+00-0.310D+00-0.571D+00 0.641D+00 0.123D+01

Coeff: 0.896D-04-0.222D-02-0.189D-02-0.425D-02 0.211D-02 0.710D-01

Coeff: 0.537D-01-0.108D+00-0.310D+00-0.571D+00 0.641D+00 0.123D+01

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=2.36D-07 MaxDP=9.96D-06 DE=-1.37D-09 OVMax= 1.88D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.67D-07 CP: 1.00D+00 1.03D+00 4.24D-01 1.01D+00 8.98D-01

CP: 1.77D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.96D+00

E= -1276.01430719021 Delta-E= -0.000000001397 Rises=F Damp=F

DIIS: error= 6.71D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1276.01430719021 IErMin=13 ErrMin= 6.71D-07

ErrMax= 6.71D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.07D-10 BMatP= 3.12D-10

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

Coeff-Com: 0.603D-04-0.973D-03-0.862D-03-0.379D-02-0.431D-02 0.163D-01

Coeff-Com: 0.310D-01 0.320D-01-0.968D-01-0.420D+00-0.174D+00 0.419D+00

Coeff-Com: 0.120D+01

Coeff: 0.603D-04-0.973D-03-0.862D-03-0.379D-02-0.431D-02 0.163D-01

Coeff: 0.310D-01 0.320D-01-0.968D-01-0.420D+00-0.174D+00 0.419D+00

Coeff: 0.120D+01

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=2.10D-07 MaxDP=8.84D-06 DE=-1.40D-09 OVMax= 1.67D-04

Cycle 14 Pass 1 IDiag 1:

RMSU= 4.13D-08 CP: 1.00D+00 1.03D+00 4.26D-01 1.02D+00 9.00D-01

CP: 1.83D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.16D+00

E= -1276.01430719082 Delta-E= -0.000000000614 Rises=F Damp=F

DIIS: error= 2.18D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1276.01430719082 IErMin=14 ErrMin= 2.18D-07

ErrMax= 2.18D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.21D-11 BMatP= 1.07D-10

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

Coeff-Com: 0.369D-05 0.324D-03 0.141D-03-0.969D-03-0.464D-02-0.220D-01

Coeff-Com: -0.590D-02 0.782D-01 0.734D-01-0.342D-01-0.366D+00-0.268D+00

Coeff-Com: 0.839D+00 0.711D+00

Coeff: 0.369D-05 0.324D-03 0.141D-03-0.969D-03-0.464D-02-0.220D-01

Coeff: -0.590D-02 0.782D-01 0.734D-01-0.342D-01-0.366D+00-0.268D+00

Coeff: 0.839D+00 0.711D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=8.52D-08 MaxDP=3.67D-06 DE=-6.14D-10 OVMax= 6.75D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 1.09D-08 CP: 1.00D+00 1.03D+00 4.27D-01 1.02D+00 9.01D-01

CP: 1.86D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.62D+00 1.41D+00

E= -1276.01430719089 Delta-E= -0.000000000071 Rises=F Damp=F

DIIS: error= 6.44D-08 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1276.01430719089 IErMin=15 ErrMin= 6.44D-08

ErrMax= 6.44D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.27D-12 BMatP= 4.21D-11

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

Coeff-Com: -0.110D-04 0.361D-03 0.265D-03 0.382D-03-0.121D-02-0.135D-01

Coeff-Com: -0.897D-02 0.285D-01 0.539D-01 0.746D-01-0.138D+00-0.213D+00

Coeff-Com: 0.127D+00 0.350D+00 0.740D+00

Coeff: -0.110D-04 0.361D-03 0.265D-03 0.382D-03-0.121D-02-0.135D-01

Coeff: -0.897D-02 0.285D-01 0.539D-01 0.746D-01-0.138D+00-0.213D+00

Coeff: 0.127D+00 0.350D+00 0.740D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=2.35D-08 MaxDP=9.81D-07 DE=-7.09D-11 OVMax= 1.84D-05

Cycle 16 Pass 1 IDiag 1:

RMSU= 3.63D-09 CP: 1.00D+00 1.03D+00 4.28D-01 1.02D+00 9.01D-01

CP: 1.86D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.75D+00 1.51D+00 1.22D+00

E= -1276.01430719090 Delta-E= -0.000000000008 Rises=F Damp=F

DIIS: error= 3.20D-08 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1276.01430719090 IErMin=16 ErrMin= 3.20D-08

ErrMax= 3.20D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.68D-12 BMatP= 6.27D-12

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

Coeff-Com: -0.713D-05 0.961D-04 0.101D-03 0.495D-03 0.706D-03-0.662D-03

Coeff-Com: -0.310D-02-0.811D-02 0.673D-02 0.500D-01 0.379D-01-0.194D-01

Coeff-Com: -0.182D+00-0.191D-01 0.357D+00 0.780D+00

Coeff: -0.713D-05 0.961D-04 0.101D-03 0.495D-03 0.706D-03-0.662D-03

Coeff: -0.310D-02-0.811D-02 0.673D-02 0.500D-01 0.379D-01-0.194D-01

Coeff: -0.182D+00-0.191D-01 0.357D+00 0.780D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=2.26D-09 MaxDP=1.35D-07 DE=-7.73D-12 OVMax= 7.47D-07

Error on total polarization charges = 0.06996

SCF Done: E(UB3LYP) = -1276.01430719 A.U. after 16 cycles

NFock= 16 Conv=0.23D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7685 S= 0.5092

<L.S>= 0.000000000000E+00

KE= 1.320977395525D+03 PE=-8.597958342509D+03 EE= 3.241797183178D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.68

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7685, after 0.7502

Leave Link 502 at Tue Sep 17 13:58:07 2019, MaxMem= 2415919104 cpu: 1563.0

(Enter /home/blab/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15309 LenP2D= 41206.

LDataN: DoStor=T MaxTD1= 6 Len= 172

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

GePol: Maximum number of non-zero 1st derivatives = 253

Leave Link 701 at Tue Sep 17 13:58:11 2019, MaxMem= 2415919104 cpu: 73.1

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 13:58:11 2019, MaxMem= 2415919104 cpu: 0.3

(Enter /home/blab/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

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

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

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

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

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Tue Sep 17 13:58:22 2019, MaxMem= 2415919104 cpu: 202.6

(Enter /home/blab/g09/l716.exe)

Dipole = 5.45341550D-13 1.75859327D-13 8.88178420D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.008627956 -0.001310421 0.000000000

2 7 -0.005628922 0.002536276 -0.000000000

3 6 0.000100754 -0.005207105 0.000000000

4 6 0.003221183 0.001320770 0.000000000

5 6 -0.002241262 0.001008556 -0.000000000

6 7 0.004492796 0.006211259 -0.000000000

7 6 -0.005674545 -0.009359384 -0.000000000

8 7 0.002456911 0.005428645 -0.000000000

9 6 -0.008299921 0.003623746 0.000000000

10 6 0.003314260 -0.005626430 -0.000000000

11 6 0.002163884 0.003574456 -0.000000000

12 7 -0.005984786 0.004884960 -0.000000000

13 6 -0.003314260 0.005626430 -0.000000000

14 6 -0.002163884 -0.003574456 0.000000000

15 6 0.005674545 0.009359384 -0.000000000

16 7 -0.002456911 -0.005428645 0.000000000

17 6 0.008299921 -0.003623746 -0.000000000

18 7 -0.004492796 -0.006211259 -0.000000000

19 7 0.005628922 -0.002536276 0.000000000

20 6 -0.000100754 0.005207105 -0.000000000

21 6 -0.003221183 -0.001320770 -0.000000000

22 6 0.002241262 -0.001008556 -0.000000000

23 6 -0.008627956 0.001310421 -0.000000000

24 7 0.005984786 -0.004884960 -0.000000000

25 30 0.000000000 0.000000000 -0.000000000

26 6 -0.000070281 -0.000485018 -0.000000000

27 1 0.000011835 0.000082032 0.000000000

28 6 0.000237876 0.000407407 -0.000000000

29 1 -0.000349066 0.000124083 0.000000000

30 6 -0.000237876 -0.000407407 0.000000000

31 1 0.000349066 -0.000124083 0.000000000

32 6 0.000070281 0.000485018 -0.000000000

33 1 -0.000011835 -0.000082032 0.000000000

34 1 -0.000125852 0.000213118 -0.000000000

35 1 0.000004835 0.000047245 0.000330293

36 1 0.000004835 0.000047245 -0.000330293

37 1 -0.000146305 0.000158752 0.000335265

38 1 -0.000146305 0.000158752 -0.000335265

39 1 -0.000155494 -0.000116481 -0.000000000

40 1 0.000146305 -0.000158752 0.000335265

41 1 0.000146305 -0.000158752 -0.000335265

42 1 0.000155494 0.000116481 -0.000000000

43 1 -0.000004835 -0.000047245 0.000330293

44 1 -0.000004835 -0.000047245 -0.000330293

45 1 0.000125852 -0.000213118 0.000000000

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

Cartesian Forces: Max 0.009359384 RMS 0.002922908

Leave Link 716 at Tue Sep 17 13:58:22 2019, MaxMem= 2415919104 cpu: 0.3

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

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

Internal Forces: Max 0.006550077 RMS 0.001109248

Search for a local minimum.

Step number 5 out of a maximum of 270

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

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4 5

DE= -5.90D-04 DEPred=-4.52D-04 R= 1.31D+00

TightC=F SS= 1.41D+00 RLast= 5.20D-02 DXNew= 5.0454D-01 1.5603D-01

Trust test= 1.31D+00 RLast= 5.20D-02 DXMaxT set to 3.00D-01

ITU= 1 0 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01333

Eigenvalues --- 0.01335 0.01336 0.01336 0.01609 0.01628

Eigenvalues --- 0.01640 0.01643 0.01770 0.01787 0.01806

Eigenvalues --- 0.01811 0.01887 0.01903 0.01938 0.01945

Eigenvalues --- 0.01997 0.01998 0.02044 0.02050 0.02070

Eigenvalues --- 0.02087 0.02101 0.02110 0.02112 0.02205

Eigenvalues --- 0.02313 0.02319 0.02352 0.02374 0.07143

Eigenvalues --- 0.07143 0.07146 0.07172 0.07172 0.07212

Eigenvalues --- 0.07285 0.07287 0.10408 0.14486 0.14504

Eigenvalues --- 0.15392 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16011 0.16026 0.16037

Eigenvalues --- 0.16175 0.16584 0.19095 0.21753 0.22075

Eigenvalues --- 0.22097 0.23853 0.23855 0.23887 0.24234

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25008 0.25053

Eigenvalues --- 0.28284 0.30155 0.33207 0.33213 0.33228

Eigenvalues --- 0.33282 0.33282 0.33397 0.33444 0.33724

Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33728 0.33755 0.34390 0.34434 0.34437

Eigenvalues --- 0.34437 0.34503 0.35539 0.35543 0.35674

Eigenvalues --- 0.35682 0.35682 0.35757 0.36832 0.38784

Eigenvalues --- 0.40938 0.41636 0.41739 0.43255 0.47656

Eigenvalues --- 0.48488 0.48943 0.49004 0.50713 0.51358

Eigenvalues --- 0.51366 0.52306 0.53800 0.53989 0.54043

Eigenvalues --- 0.54887 0.56314 0.56357 0.58449

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 1.43740 -0.43740

Cosine: 1.000 > 0.970

Length: 1.000

GDIIS step was calculated using 2 of the last 5 vectors.

Iteration 1 RMS(Cart)= 0.00770968 RMS(Int)= 0.00003145

Iteration 2 RMS(Cart)= 0.00005358 RMS(Int)= 0.00000524

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000524

ITry= 1 IFail=0 DXMaxC= 2.97D-02 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.07D-09 for atom 29.

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

(Linear) (Quad) (Total)

R1 2.61150 -0.00407 -0.00437 -0.01178 -0.01615 2.59535

R2 2.71649 -0.00038 0.00511 -0.00702 -0.00191 2.71458

R3 2.55238 0.00450 -0.00171 0.02243 0.02072 2.57311

R4 2.55851 0.00306 0.00285 0.00964 0.01250 2.57101

R5 3.80610 -0.00120 -0.00232 -0.01517 -0.01750 3.78860

R6 2.75052 -0.00221 0.00405 -0.01680 -0.01277 2.73775

R7 2.57769 0.00047 -0.00552 0.01310 0.00759 2.58528

R8 2.61195 0.00189 -0.00257 0.01184 0.00927 2.62122

R9 2.82242 0.00011 -0.00040 0.00011 -0.00029 2.82213

R10 2.04598 -0.00005 -0.00009 0.00018 0.00010 2.04608

R11 2.53519 -0.00655 -0.00063 -0.02912 -0.02975 2.50544

R12 2.56243 0.00314 0.00246 0.01033 0.01279 2.57522

R13 2.76866 0.00146 -0.00105 0.01506 0.01400 2.78266

R14 2.61344 -0.00344 -0.00460 -0.00881 -0.01340 2.60004

R15 3.79860 -0.00110 -0.00154 -0.02124 -0.02278 3.77583

R16 2.77189 0.00401 0.00221 0.02978 0.03200 2.80389

R17 2.50139 -0.00278 0.00354 -0.01662 -0.01308 2.48831

R18 2.58203 -0.00275 0.00054 -0.01649 -0.01594 2.56609

R19 2.81787 -0.00003 0.00045 -0.00220 -0.00174 2.81613

R20 2.04538 -0.00028 -0.00011 -0.00026 -0.00037 2.04501

R21 2.50139 -0.00278 0.00354 -0.01662 -0.01308 2.48831

R22 2.58203 -0.00275 0.00054 -0.01649 -0.01594 2.56609

R23 2.77189 0.00401 0.00221 0.02978 0.03200 2.80389

R24 2.81787 -0.00003 0.00045 -0.00220 -0.00174 2.81613

R25 2.76866 0.00146 -0.00105 0.01506 0.01400 2.78266

R26 2.04538 -0.00028 -0.00011 -0.00026 -0.00037 2.04501

R27 2.56243 0.00314 0.00246 0.01033 0.01279 2.57522

R28 2.53519 -0.00655 -0.00063 -0.02912 -0.02975 2.50544

R29 2.61344 -0.00344 -0.00460 -0.00881 -0.01340 2.60004

R30 3.79860 -0.00110 -0.00154 -0.02124 -0.02278 3.77583

R31 2.57769 0.00047 -0.00552 0.01310 0.00759 2.58528

R32 2.55851 0.00306 0.00285 0.00964 0.01250 2.57101

R33 2.61150 -0.00407 -0.00437 -0.01178 -0.01615 2.59535

R34 3.80610 -0.00120 -0.00232 -0.01517 -0.01750 3.78860

R35 2.75052 -0.00221 0.00405 -0.01680 -0.01277 2.73775

R36 2.61195 0.00189 -0.00257 0.01184 0.00927 2.62122

R37 2.82242 0.00011 -0.00040 0.00011 -0.00029 2.82213

R38 2.71649 -0.00038 0.00511 -0.00702 -0.00191 2.71458

R39 2.04598 -0.00005 -0.00009 0.00018 0.00010 2.04608

R40 2.55238 0.00450 -0.00171 0.02243 0.02072 2.57311

R41 2.06473 -0.00003 -0.00001 0.00087 0.00086 2.06560

R42 2.06977 0.00026 0.00069 0.00270 0.00340 2.07317

R43 2.06977 0.00026 0.00069 0.00270 0.00340 2.07317

R44 2.06816 0.00032 0.00092 0.00325 0.00417 2.07234

R45 2.06816 0.00032 0.00092 0.00325 0.00417 2.07234

R46 2.06309 -0.00000 0.00023 0.00041 0.00064 2.06373

R47 2.06816 0.00032 0.00092 0.00325 0.00417 2.07234

R48 2.06816 0.00032 0.00092 0.00325 0.00417 2.07234

R49 2.06309 -0.00000 0.00023 0.00041 0.00064 2.06373

R50 2.06977 0.00026 0.00069 0.00270 0.00340 2.07317

R51 2.06977 0.00026 0.00069 0.00270 0.00340 2.07317

R52 2.06473 -0.00003 -0.00001 0.00087 0.00086 2.06560

A1 1.88078 0.00046 0.00159 0.00942 0.01103 1.89180

A2 2.20175 0.00040 0.00188 -0.00600 -0.00413 2.19762

A3 2.20066 -0.00086 -0.00347 -0.00342 -0.00690 2.19376

A4 1.90809 0.00047 -0.00054 -0.01136 -0.01189 1.89620

A5 2.18217 0.00006 0.00125 0.00397 0.00520 2.18737

A6 2.19292 -0.00053 -0.00071 0.00740 0.00669 2.19961

A7 1.89803 -0.00044 -0.00020 0.01097 0.01076 1.90878

A8 2.22694 -0.00067 -0.00083 -0.01340 -0.01422 2.21273

A9 2.15821 0.00112 0.00103 0.00242 0.00346 2.16167

A10 1.85430 -0.00042 -0.00019 -0.00673 -0.00694 1.84735

A11 2.17830 0.00075 0.00013 0.01382 0.01396 2.19226

A12 2.25059 -0.00033 0.00006 -0.00709 -0.00702 2.24357

A13 1.88359 -0.00007 -0.00066 -0.00230 -0.00296 1.88063

A14 2.18225 -0.00003 -0.00030 0.00520 0.00490 2.18716

A15 2.21734 0.00010 0.00096 -0.00290 -0.00194 2.21540

A16 2.15840 0.00083 0.00265 0.00211 0.00477 2.16317

A17 2.22777 0.00071 -0.00087 0.00279 0.00192 2.22969

A18 2.16735 0.00030 0.00186 -0.00608 -0.00422 2.16313

A19 1.88806 -0.00101 -0.00098 0.00329 0.00230 1.89036

A20 1.90886 0.00031 0.00062 -0.00342 -0.00281 1.90605

A21 2.20027 -0.00052 -0.00162 0.00260 0.00096 2.20124

A22 2.17405 0.00020 0.00101 0.00083 0.00184 2.17589

A23 1.88467 0.00019 0.00101 0.00040 0.00141 1.88608

A24 2.22320 0.00140 0.00103 0.00622 0.00726 2.23046

A25 2.17531 -0.00159 -0.00204 -0.00662 -0.00866 2.16665

A26 1.86175 -0.00021 -0.00157 0.00098 -0.00059 1.86116

A27 2.17638 -0.00082 -0.00053 -0.00631 -0.00685 2.16953

A28 2.24505 0.00103 0.00211 0.00534 0.00744 2.25250

A29 1.88143 0.00072 0.00093 -0.00124 -0.00031 1.88112

A30 2.17886 -0.00060 -0.00115 -0.00148 -0.00263 2.17623

A31 2.22289 -0.00011 0.00023 0.00272 0.00294 2.22583

A32 2.20366 -0.00189 -0.00378 -0.00651 -0.01029 2.19337

A33 1.86175 -0.00021 -0.00157 0.00098 -0.00059 1.86116

A34 2.24505 0.00103 0.00211 0.00534 0.00744 2.25250

A35 2.17638 -0.00082 -0.00053 -0.00631 -0.00685 2.16953

A36 1.88143 0.00072 0.00093 -0.00124 -0.00031 1.88112

A37 2.22289 -0.00011 0.00023 0.00272 0.00294 2.22583

A38 2.17886 -0.00060 -0.00115 -0.00148 -0.00263 2.17623

A39 1.88806 -0.00101 -0.00098 0.00329 0.00230 1.89036

A40 2.16735 0.00030 0.00186 -0.00608 -0.00422 2.16313

A41 2.22777 0.00071 -0.00087 0.00279 0.00192 2.22969

A42 1.90886 0.00031 0.00062 -0.00342 -0.00281 1.90605

A43 2.20027 -0.00052 -0.00162 0.00260 0.00096 2.20124

A44 2.17405 0.00020 0.00101 0.00083 0.00184 2.17589

A45 2.17531 -0.00159 -0.00204 -0.00662 -0.00866 2.16665

A46 2.22320 0.00140 0.00103 0.00622 0.00726 2.23046

A47 1.88467 0.00019 0.00101 0.00040 0.00141 1.88608

A48 2.15840 0.00083 0.00265 0.00211 0.00477 2.16317

A49 1.90809 0.00047 -0.00054 -0.01136 -0.01189 1.89620

A50 2.19292 -0.00053 -0.00071 0.00740 0.00669 2.19961

A51 2.18217 0.00006 0.00125 0.00397 0.00520 2.18737

A52 2.22694 -0.00067 -0.00083 -0.01340 -0.01422 2.21273

A53 2.15821 0.00112 0.00103 0.00242 0.00346 2.16167

A54 1.89803 -0.00044 -0.00020 0.01097 0.01076 1.90878

A55 1.85430 -0.00042 -0.00019 -0.00673 -0.00694 1.84735

A56 2.17830 0.00075 0.00013 0.01382 0.01396 2.19226

A57 2.25059 -0.00033 0.00006 -0.00709 -0.00702 2.24357

A58 1.88359 -0.00007 -0.00066 -0.00230 -0.00296 1.88063

A59 2.21734 0.00010 0.00096 -0.00290 -0.00194 2.21540

A60 2.18225 -0.00003 -0.00030 0.00520 0.00490 2.18716

A61 1.88078 0.00046 0.00159 0.00942 0.01103 1.89180

A62 2.20175 0.00040 0.00188 -0.00600 -0.00413 2.19762

A63 2.20066 -0.00086 -0.00347 -0.00342 -0.00690 2.19376

A64 2.20366 -0.00189 -0.00378 -0.00651 -0.01029 2.19337

A65 1.56006 0.00018 0.00138 -0.00150 -0.00012 1.55993

A66 1.58154 -0.00018 -0.00138 0.00150 0.00012 1.58166

A67 1.58154 -0.00018 -0.00138 0.00150 0.00012 1.58166

A68 1.56006 0.00018 0.00138 -0.00150 -0.00012 1.55993

A69 1.94638 -0.00034 -0.00135 -0.00347 -0.00484 1.94154

A70 1.94923 -0.00009 -0.00133 -0.00038 -0.00172 1.94751

A71 1.94923 -0.00009 -0.00133 -0.00038 -0.00172 1.94751

A72 1.88073 0.00015 0.00115 -0.00038 0.00076 1.88149

A73 1.88073 0.00015 0.00115 -0.00038 0.00076 1.88149

A74 1.85306 0.00026 0.00204 0.00540 0.00743 1.86049

A75 1.94290 -0.00023 -0.00053 -0.00363 -0.00416 1.93874

A76 1.94290 -0.00023 -0.00053 -0.00363 -0.00416 1.93874

A77 1.94521 -0.00017 -0.00101 -0.00194 -0.00295 1.94226

A78 1.85604 0.00024 0.00143 0.00307 0.00450 1.86054

A79 1.88660 0.00022 0.00040 0.00335 0.00374 1.89034

A80 1.88660 0.00022 0.00040 0.00335 0.00374 1.89034

A81 1.94290 -0.00023 -0.00053 -0.00363 -0.00416 1.93874

A82 1.94290 -0.00023 -0.00053 -0.00363 -0.00416 1.93874

A83 1.94521 -0.00017 -0.00101 -0.00194 -0.00295 1.94226

A84 1.85604 0.00024 0.00143 0.00307 0.00450 1.86054

A85 1.88660 0.00022 0.00040 0.00335 0.00374 1.89034

A86 1.88660 0.00022 0.00040 0.00335 0.00374 1.89034

A87 1.94923 -0.00009 -0.00133 -0.00038 -0.00172 1.94751

A88 1.94923 -0.00009 -0.00133 -0.00038 -0.00172 1.94751

A89 1.94638 -0.00034 -0.00135 -0.00347 -0.00484 1.94154

A90 1.85306 0.00026 0.00204 0.00540 0.00743 1.86049

A91 1.88073 0.00015 0.00115 -0.00038 0.00076 1.88149

A92 1.88073 0.00015 0.00115 -0.00038 0.00076 1.88149

A93 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

A94 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

A95 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

A96 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D2 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D3 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D4 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D6 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D7 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D10 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D11 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D12 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D13 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D14 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D15 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D16 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D17 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D18 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D19 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D20 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D21 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D22 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D23 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D24 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D25 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D26 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D27 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D28 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D29 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D30 1.03610 0.00011 0.00040 0.00317 0.00356 1.03965

D31 -1.03610 -0.00011 -0.00040 -0.00317 -0.00356 -1.03965

D32 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.10550 0.00011 0.00040 0.00317 0.00356 -2.10194

D34 2.10550 -0.00011 -0.00040 -0.00317 -0.00356 2.10194

D35 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D36 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D37 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D38 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D39 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D40 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D41 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D42 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D43 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D44 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D45 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D46 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D47 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D48 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D49 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D50 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D51 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D52 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D53 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D54 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D55 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D56 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D57 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D58 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D59 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D60 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D61 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D62 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D63 1.03378 -0.00000 0.00055 -0.00044 0.00011 1.03389

D64 -1.03378 0.00000 -0.00055 0.00044 -0.00011 -1.03389

D65 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D66 -2.10782 -0.00000 0.00055 -0.00044 0.00011 -2.10770

D67 2.10782 0.00000 -0.00055 0.00044 -0.00011 2.10770

D68 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D69 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D70 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D71 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D72 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D73 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D74 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D75 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D76 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D77 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D78 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D79 -2.10782 -0.00000 0.00055 -0.00044 0.00011 -2.10770

D80 2.10782 0.00000 -0.00055 0.00044 -0.00011 2.10770

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 1.03378 -0.00000 0.00055 -0.00044 0.00011 1.03389

D83 -1.03378 0.00000 -0.00055 0.00044 -0.00011 -1.03389

D84 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D85 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D86 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D87 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D88 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D89 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D90 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D91 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D92 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D93 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D94 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D95 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D96 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D97 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D98 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D99 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D100 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D101 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D102 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D103 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D104 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D105 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D106 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D107 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D108 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D109 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D110 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D111 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D112 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D113 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D114 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D116 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D117 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D118 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D119 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D120 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D121 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D122 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D123 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D124 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D125 1.03610 0.00011 0.00040 0.00317 0.00356 1.03965

D126 -1.03610 -0.00011 -0.00040 -0.00317 -0.00356 -1.03965

D127 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D128 -2.10550 0.00011 0.00040 0.00317 0.00356 -2.10194

D129 2.10550 -0.00011 -0.00040 -0.00317 -0.00356 2.10194

D130 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D131 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D132 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D133 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D134 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D135 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D136 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

Item Value Threshold Converged?

Maximum Force 0.006550 0.000450 NO

RMS Force 0.001109 0.000300 NO

Maximum Displacement 0.029678 0.001800 NO

RMS Displacement 0.007714 0.001200 NO

Predicted change in Energy=-9.022794D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 13:58:22 2019, MaxMem= 2415919104 cpu: 1.6

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

Input orientation:

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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1 6 0 -2.066592 -2.195253 -0.000000

2 7 0 -0.733259 -1.865935 -0.000000

3 6 0 -0.001889 -3.013152 -0.000000

4 6 0 -0.896150 -4.152970 -0.000000

5 6 0 -2.179765 -3.627282 -0.000000

6 7 0 1.362400 -3.114819 -0.000000

7 6 0 2.182337 -2.072944 -0.000000

8 7 0 1.851598 -0.750942 -0.000000

9 6 0 3.002164 0.003540 -0.000000

10 6 0 4.160439 -0.923783 -0.000000

11 6 0 3.650780 -2.182427 -0.000000

12 7 0 -3.106419 -1.316166 -0.000000

13 6 0 -4.160439 0.923783 -0.000000

14 6 0 -3.650780 2.182427 -0.000000

15 6 0 -2.182337 2.072944 -0.000000

16 7 0 -1.851598 0.750942 -0.000000

17 6 0 -3.002164 -0.003540 -0.000000

18 7 0 -1.362400 3.114819 -0.000000

19 7 0 0.733259 1.865935 -0.000000

20 6 0 0.001889 3.013152 -0.000000

21 6 0 0.896150 4.152970 -0.000000

22 6 0 2.179765 3.627282 -0.000000

23 6 0 2.066592 2.195253 -0.000000

24 7 0 3.106419 1.316166 -0.000000

25 30 0 0.000000 -0.000000 -0.000000

26 6 0 -0.477599 -5.586525 -0.000000

27 1 0 -3.109830 -4.181627 -0.000000

28 6 0 5.585445 -0.487729 -0.000000

29 1 0 4.198801 -3.115577 -0.000000

30 6 0 -5.585445 0.487729 -0.000000

31 1 0 -4.198801 3.115577 -0.000000

32 6 0 0.477599 5.586525 -0.000000

33 1 0 3.109830 4.181627 -0.000000

34 1 0 -1.344576 -6.252218 -0.000000

35 1 0 0.131526 -5.829110 0.879598

36 1 0 0.131526 -5.829110 -0.879598

37 1 0 5.809499 0.128152 0.879259

38 1 0 5.809499 0.128152 -0.879259

39 1 0 6.262254 -1.344796 -0.000000

40 1 0 -5.809499 -0.128152 0.879259

41 1 0 -5.809499 -0.128152 -0.879259

42 1 0 -6.262254 1.344796 -0.000000

43 1 0 -0.131526 5.829110 0.879598

44 1 0 -0.131526 5.829110 -0.879598

45 1 0 1.344576 6.252218 -0.000000

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Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.373400 0.000000

3 C 2.220801 1.360518 0.000000

4 C 2.280919 2.292829 1.448755 0.000000

5 C 1.436494 2.279194 2.262809 1.387089 0.000000

6 N 3.550153 2.439569 1.368072 2.485721 3.579044

7 C 4.250689 2.922936 2.377989 3.715319 4.630757

8 N 4.175913 2.815083 2.924552 4.373090 4.952295

9 C 5.525123 4.177119 4.257319 5.698546 6.327342

10 C 6.355514 4.983566 4.657299 5.999729 6.892539

11 C 5.717387 4.395448 3.745944 4.955564 6.006902

12 N 1.361629 2.436008 3.538060 3.596213 2.489969

13 C 3.756671 4.419060 5.726517 6.035644 4.963392

14 C 4.655506 4.990107 6.348894 6.908346 5.993047

15 C 4.269766 4.196975 5.533781 6.357381 5.700227

16 N 2.954029 2.845827 4.194023 4.996122 4.390506

17 C 2.383045 2.935379 4.249638 4.653286 3.715892

18 N 5.356562 5.020332 6.277183 7.282730 6.791467

19 N 4.932790 4.009680 4.934160 6.235559 6.217809

20 C 5.604114 4.934160 6.026305 7.222173 6.989634

21 C 7.005554 6.235559 7.222173 8.497117 8.366217

22 C 7.206488 6.217809 6.989634 8.366217 8.463700

23 C 6.029905 4.932790 5.604114 7.005554 7.206488

24 N 6.252208 4.986872 5.329593 6.777315 7.237501

25 Zn 3.014953 2.004840 3.013153 4.248558 4.231850

26 C 3.745080 3.729363 2.616973 1.493407 2.595381

27 H 2.243664 3.318210 3.320336 2.213865 1.082737

28 C 7.840237 6.467262 6.131563 7.446145 8.375875

29 H 6.332626 5.087909 4.201938 5.199492 6.399059

30 C 4.425010 5.392907 6.590316 6.597391 5.341532

31 H 5.722870 6.068398 7.428014 7.983689 7.038655

32 C 8.187123 7.550188 8.613034 9.835901 9.589360

33 H 8.213401 7.165357 7.838854 9.247345 9.431802

34 H 4.120713 4.428678 3.506331 2.146608 2.754602

35 H 4.337088 4.150698 2.953153 2.153893 3.311163

36 H 4.337088 4.150698 2.953153 2.153893 3.311163

37 H 8.258579 6.896170 6.664317 8.004176 8.871569

38 H 8.258579 6.896170 6.664317 8.004176 8.871569

39 H 8.372154 7.014898 6.482507 7.689513 8.745138

40 H 4.365244 5.437021 6.544055 6.411962 5.117810

41 H 4.365244 5.437021 6.544055 6.411962 5.117810

42 H 5.489584 6.393636 7.627836 7.682480 6.433372

43 H 8.301119 7.768494 8.886849 10.049889 9.715572

44 H 8.301119 7.768494 8.886849 10.049889 9.715572

45 H 9.110205 8.379846 9.362695 10.643721 10.489305

6 7 8 9 10

6 N 0.000000

7 C 1.325821 0.000000

8 N 2.413966 1.362747 0.000000

9 C 3.523207 2.232465 1.375880 0.000000

10 C 3.553824 2.287675 2.315301 1.483755 0.000000

11 C 2.471040 1.472519 2.299175 2.280165 1.357917

12 N 4.817208 5.342626 4.990131 6.249512 7.277443

13 C 6.841934 7.015068 6.240937 7.221477 8.523527

14 C 7.293339 7.220349 6.235449 7.000659 8.406169

15 C 6.283156 6.019865 4.924121 5.582248 7.015068

16 N 5.027315 4.924121 3.996163 4.910969 6.240937

17 C 5.359989 5.582248 4.910969 6.004333 7.221477

18 N 6.799480 6.283156 5.027315 5.359989 6.841934

19 N 5.020332 4.196975 2.845827 2.935379 4.419060

20 C 6.277183 5.533781 4.194023 4.249638 5.726517

21 C 7.282730 6.357381 4.996122 4.653286 6.035644

22 C 6.791467 5.700227 4.390506 3.715892 4.963392

23 C 5.356562 4.269766 2.954029 2.383045 3.756671

24 N 4.761851 3.512832 2.418162 1.316759 2.475546

25 Zn 3.399740 3.009932 1.998081 3.002166 4.261763

26 C 3.081384 4.406871 5.367310 6.584647 6.576668

27 H 4.597708 5.696804 6.032029 7.407570 7.966829

28 C 4.973501 3.754204 3.743113 2.629579 1.490230

29 H 2.836401 2.270068 3.331796 3.340783 2.192130

30 C 7.826295 8.178966 7.539490 8.601248 9.847569

31 H 8.351335 8.224335 7.180341 7.844659 9.284036

32 C 8.746214 7.846885 6.484702 6.127247 7.479801

33 H 7.502776 6.322966 5.090519 4.179474 5.212388

34 H 4.143790 5.468587 6.362355 7.617654 7.661424

35 H 3.107430 4.369016 5.433243 6.560035 6.408438

36 H 3.107430 4.369016 5.433243 6.560035 6.408438

37 H 5.573746 4.332923 4.148600 2.944445 2.144543

38 H 5.573746 4.332923 4.148600 2.944445 2.144543

39 H 5.209756 4.144385 4.450455 3.527917 2.143567

40 H 7.818530 8.271926 7.736496 8.856402 10.040209

41 H 7.818530 8.271926 7.736496 8.856402 10.040209

42 H 8.833092 9.109999 8.380138 9.361005 10.666723

43 H 9.110399 8.280707 6.928460 6.673153 8.049609

44 H 9.110399 8.280707 6.928460 6.673153 8.049609

45 H 9.367054 8.367208 7.021490 6.464796 7.708701

11 12 13 14 15

11 C 0.000000

12 N 6.812499 0.000000

13 C 8.406169 2.475546 0.000000

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16 N 6.235449 2.418162 2.315301 2.299175 1.362747

17 C 7.000659 1.316759 1.483755 2.280165 2.232465

18 N 7.293339 4.761851 3.553824 2.471040 1.325821

19 N 4.990107 4.986872 4.983566 4.395448 2.922936

20 C 6.348894 5.329593 4.657299 3.745944 2.377989

21 C 6.908346 6.777315 5.999729 4.955564 3.715319

22 C 5.993047 7.237501 6.892539 6.006902 4.630757

23 C 4.655506 6.252208 6.355514 5.717387 4.250689

24 N 3.540689 6.747482 7.277443 6.812499 5.342626

25 Zn 4.253373 3.373741 4.261763 4.253373 3.009932

26 C 5.350831 5.014645 7.479801 8.392002 7.846885

27 H 7.050011 2.865464 5.212388 6.387003 6.322966

28 C 2.571951 8.731254 9.847569 9.614447 8.178966

29 H 1.082172 7.523571 9.284036 9.470205 8.224335

30 C 9.614447 3.065878 1.490230 2.571951 3.754204

31 H 9.470205 4.564389 2.192130 1.082172 2.270068

32 C 8.392002 7.777681 6.576668 5.350831 4.406871

33 H 6.387003 8.298643 7.966829 7.050011 5.696804

34 H 6.443352 5.241060 7.708701 8.744245 8.367208

35 H 5.143651 5.623579 8.049609 8.903047 8.280707

36 H 5.143651 5.623579 8.049609 8.903047 8.280707

37 H 3.282063 9.074841 10.040209 9.720598 8.271926

38 H 3.282063 9.074841 10.040209 9.720598 8.271926

39 H 2.742521 9.368717 10.666723 10.521861 9.109999

40 H 9.720598 3.080766 2.144543 3.282063 4.332923

41 H 9.720598 3.080766 2.144543 3.282063 4.332923

42 H 10.521861 4.127955 2.143567 2.742521 4.144385

43 H 8.903047 7.789650 6.408438 5.143651 4.369016

44 H 8.903047 7.789650 6.408438 5.143651 4.369016

45 H 8.744245 8.780193 7.661424 6.443352 5.468587

16 17 18 19 20

16 N 0.000000

17 C 1.375880 0.000000

18 N 2.413966 3.523207 0.000000

19 N 2.815083 4.177119 2.439569 0.000000

20 C 2.924552 4.257319 1.368072 1.360518 0.000000

21 C 4.373090 5.698546 2.485721 2.292829 1.448755

22 C 4.952295 6.327342 3.579044 2.279194 2.262809

23 C 4.175913 5.525123 3.550153 1.373400 2.220801

24 N 4.990131 6.249512 4.817208 2.436008 3.538060

25 Zn 1.998081 3.002166 3.399740 2.004840 3.013153

26 C 6.484702 6.127247 8.746214 7.550188 8.613034

27 H 5.090519 4.179474 7.502776 7.165357 7.838854

28 C 7.539490 8.601248 7.826295 5.392907 6.590316

29 H 7.180341 7.844659 8.351335 6.068398 7.428014

30 C 3.743113 2.629579 4.973501 6.467262 6.131563

31 H 3.331796 3.340783 2.836401 5.087909 4.201938

32 C 5.367310 6.584647 3.081384 3.729363 2.616973

33 H 6.032029 7.407570 4.597708 3.318210 3.320336

34 H 7.021490 6.464796 9.367054 8.379846 9.362695

35 H 6.928460 6.673153 9.110399 7.768494 8.886849

36 H 6.928460 6.673153 9.110399 7.768494 8.886849

37 H 7.736496 8.856402 7.818530 5.437021 6.544055

38 H 7.736496 8.856402 7.818530 5.437021 6.544055

39 H 8.380138 9.361005 8.833092 6.393636 7.627836

40 H 4.148600 2.944445 5.573746 6.896170 6.664317

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42 H 4.450455 3.527917 5.209756 7.014898 6.482507

43 H 5.433243 6.560035 3.107430 4.150698 2.953153

44 H 5.433243 6.560035 3.107430 4.150698 2.953153

45 H 6.362355 7.617654 4.143790 4.428678 3.506331

21 22 23 24 25

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22 C 1.387089 0.000000

23 C 2.280919 1.436494 0.000000

24 N 3.596213 2.489969 1.361629 0.000000

25 Zn 4.248558 4.231850 3.014953 3.373741 0.000000

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27 H 9.247345 9.431802 8.213401 8.298643 5.211242

28 C 6.597391 5.341532 4.425010 3.065878 5.606699

29 H 7.983689 7.038655 5.722870 4.564389 5.228456

30 C 7.446145 8.375875 7.840237 8.731254 5.606699

31 H 5.199492 6.399059 6.332626 7.523571 5.228456

32 C 1.493407 2.595381 3.745080 5.014645 5.606903

33 H 2.213865 1.082737 2.243664 2.865464 5.211242

34 H 10.643721 10.489305 9.110205 8.780193 6.395164

35 H 10.049889 9.715572 8.301119 7.789650 5.896568

36 H 10.049889 9.715572 8.301119 7.789650 5.896568

37 H 6.411962 5.117810 4.365244 3.080766 5.877057

38 H 6.411962 5.117810 4.365244 3.080766 5.877057

39 H 7.682480 6.433372 5.489584 4.127955 6.405022

40 H 8.004176 8.871569 8.258579 9.074841 5.877057

41 H 8.004176 8.871569 8.258579 9.074841 5.877057

42 H 7.689513 8.745138 8.372154 9.368717 6.405022

43 H 2.153893 3.311163 4.337088 5.623579 5.896568

44 H 2.153893 3.311163 4.337088 5.623579 5.896568

45 H 2.146608 2.754602 4.120713 5.241060 6.395164

26 27 28 29 30

26 C 0.000000

27 H 2.983686 0.000000

28 C 7.922009 9.447364 0.000000

29 H 5.289073 7.385970 2.971257 0.000000

30 C 7.936413 5.285031 11.213398 10.426662 0.000000

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32 C 11.213806 10.406077 7.936413 9.464351 7.922009

33 H 10.406077 10.422485 5.285031 7.378011 9.447364

34 H 1.093068 2.720932 9.014129 6.369266 7.963156

35 H 1.097075 3.740893 7.684353 4.967865 8.565039

36 H 1.097075 3.740893 7.684353 4.967865 8.565039

37 H 8.541559 9.944935 1.096634 3.726825 11.434472

38 H 8.541559 9.944935 1.096634 3.726825 11.434472

39 H 7.963535 9.792016 1.092078 2.719101 11.988583

40 H 7.680891 4.948936 11.434472 10.481597 1.096634

41 H 7.680891 4.948936 11.434472 10.481597 1.096634

42 H 9.028037 6.362321 11.988583 11.372274 1.092078

43 H 11.454701 10.481357 8.565039 9.976615 7.684353

44 H 11.454701 10.481357 8.565039 9.976615 7.684353

45 H 11.978154 11.344905 7.963156 9.792967 9.014129

31 32 33 34 35

31 H 0.000000

32 C 5.289073 0.000000

33 H 7.385970 2.983686 0.000000

34 H 9.792967 11.978154 11.344905 0.000000

35 H 9.976615 11.454701 10.481357 1.769630 0.000000

36 H 9.976615 11.454701 10.481357 1.769630 1.759197

37 H 10.481597 7.680891 4.948936 9.626163 8.229724

38 H 10.481597 7.680891 4.948936 9.626163 8.415577

39 H 11.372274 9.028037 6.362321 9.052440 7.646477

40 H 3.726825 8.541559 9.944935 7.629733 8.233875

41 H 3.726825 8.541559 9.944935 7.629733 8.419636

42 H 2.719101 7.963535 9.792016 9.049762 9.649821

43 H 4.967865 1.097075 3.740893 12.173893 11.661187

44 H 4.967865 1.097075 3.740893 12.173893 11.793136

45 H 6.369266 1.093068 2.720932 12.790327 12.173893

36 37 38 39 40

36 H 0.000000

37 H 8.415577 0.000000

38 H 8.229724 1.758518 0.000000

39 H 7.646477 1.774164 1.774164 0.000000

40 H 8.419636 11.621825 11.754114 12.164726 0.000000

41 H 8.233875 11.754114 11.621825 12.164726 1.758518

42 H 9.649821 12.164726 12.164726 12.810044 1.774164

43 H 11.793136 8.233875 8.419636 9.649821 8.229724

44 H 11.661187 8.419636 8.233875 9.649821 8.415577

45 H 12.173893 7.629733 7.629733 9.049762 9.626163

41 42 43 44 45

41 H 0.000000

42 H 1.774164 0.000000

43 H 8.415577 7.646477 0.000000

44 H 8.229724 7.646477 1.759197 0.000000

45 H 9.626163 9.052440 1.769630 1.769630 0.000000

Stoichiometry C20H16N8Zn(1-,2)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=3 Diff= 8.63D-01

Largest Abelian subgroup C2H NOp 4

Largest concise Abelian subgroup C2H NOp 4

Standard orientation:

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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3 6 0 -1.209210 -2.759873 0.000000

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17 6 0 -2.751981 1.199834 0.000000

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28 6 0 4.921897 -2.685146 0.000000

29 1 0 2.598388 -4.537084 0.000000

30 6 0 -4.921897 2.685146 0.000000

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36 1 0 -2.215435 -5.393299 -0.879598

37 1 0 5.373980 -2.210666 0.879259

38 1 0 5.373980 -2.210666 -0.879259

39 1 0 5.198527 -3.741607 0.000000

40 1 0 -5.373980 2.210666 0.879259

41 1 0 -5.373980 2.210666 -0.879259

42 1 0 -5.198527 3.741607 0.000000

43 1 0 2.215435 5.393299 0.879598

44 1 0 2.215435 5.393299 -0.879598

45 1 0 3.737384 5.189420 0.000000

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

Rotational constants (GHZ): 0.1831498 0.1817959 0.0914410

Leave Link 202 at Tue Sep 17 13:58:22 2019, MaxMem= 2415919104 cpu: 0.2

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 229 symmetry adapted cartesian basis functions of AG symmetry.

There are 82 symmetry adapted cartesian basis functions of BG symmetry.

There are 78 symmetry adapted cartesian basis functions of AU symmetry.

There are 218 symmetry adapted cartesian basis functions of BU symmetry.

There are 212 symmetry adapted basis functions of AG symmetry.

There are 82 symmetry adapted basis functions of BG symmetry.

There are 78 symmetry adapted basis functions of AU symmetry.

There are 204 symmetry adapted basis functions of BU symmetry.

576 basis functions, 1015 primitive gaussians, 607 cartesian basis functions

103 alpha electrons 102 beta electrons

nuclear repulsion energy 2762.0818126651 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= 45 NActive= 45 NUniq= 21 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1141486134 Hartrees.

Nuclear repulsion after empirical dispersion term = 2761.9676640517 Hartrees.

No density basis found on file 724.

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

Polarizable Continuum Model (PCM)

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

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

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 = 45

GePol: Total number of spheres = 45

GePol: Number of exposed spheres = 45 (100.00%)

GePol: Number of points = 3570

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.51D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 236

GePol: Fraction of low-weight points (<1% of avg) = 6.61%

GePol: Cavity surface area = 378.398 Ang\*\*2

GePol: Cavity volume = 377.584 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0106148656 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2761.9570491861 Hartrees.

Leave Link 301 at Tue Sep 17 13:58:23 2019, MaxMem= 2415919104 cpu: 2.2

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15337 LenP2D= 41280.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.78D-04 NBF= 212 82 78 204

NBsUse= 576 1.00D-06 EigRej= -1.00D+00 NBFU= 212 82 78 204

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= 594 594 594 594 594 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Tue Sep 17 13:58:23 2019, MaxMem= 2415919104 cpu: 13.3

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 13:58:24 2019, MaxMem= 2415919104 cpu: 1.8

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

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

B after Tr= -0.000000 -0.000000 0.000000

Rot= 0.952311 -0.000000 -0.000000 -0.305129 Ang= -35.53 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-BG.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7685 S= 0.5092

Generating alternative initial guess.

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -1276.41190303506

Leave Link 401 at Tue Sep 17 13:58:26 2019, MaxMem= 2415919104 cpu: 39.5

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1141655 IEndB= 1141655 NGot= 2415919104 MDV= 2415163146

LenX= 2415163146 LenY= 2414794090

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= 670000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 38234700.

Iteration 1 A\*A^-1 deviation from unit magnitude is 9.66D-15 for 3554.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.78D-15 for 3566 1321.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.21D-15 for 3554.

Iteration 1 A^-1\*A deviation from orthogonality is 8.42D-14 for 1993 1970.

E= -1276.01384986377

DIIS: error= 1.41D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1276.01384986377 IErMin= 1 ErrMin= 1.41D-03

ErrMax= 1.41D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.47D-03 BMatP= 4.47D-03

IDIUse=3 WtCom= 9.86D-01 WtEn= 1.41D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.293 Goal= None Shift= 0.000

Gap= 0.342 Goal= None Shift= 0.000

GapD= 0.293 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.

RMSDP=1.21D-04 MaxDP=3.19D-03 OVMax= 5.44D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.21D-04 CP: 1.00D+00

E= -1276.01551989305 Delta-E= -0.001670029277 Rises=F Damp=F

DIIS: error= 6.92D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1276.01551989305 IErMin= 2 ErrMin= 6.92D-04

ErrMax= 6.92D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.69D-04 BMatP= 4.47D-03

IDIUse=3 WtCom= 9.93D-01 WtEn= 6.92D-03

Coeff-Com: 0.765D-01 0.923D+00

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

Coeff: 0.760D-01 0.924D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=5.00D-05 MaxDP=1.84D-03 DE=-1.67D-03 OVMax= 3.43D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 4.48D-05 CP: 1.00D+00 1.18D+00

E= -1276.01561999951 Delta-E= -0.000100106465 Rises=F Damp=F

DIIS: error= 5.95D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1276.01561999951 IErMin= 3 ErrMin= 5.95D-04

ErrMax= 5.95D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.28D-04 BMatP= 3.69D-04

IDIUse=3 WtCom= 2.91D-01 WtEn= 7.09D-01

Coeff-Com: -0.529D-02 0.555D+00 0.451D+00

Coeff-En: 0.000D+00 0.136D+00 0.864D+00

Coeff: -0.154D-02 0.258D+00 0.744D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=4.21D-05 MaxDP=1.59D-03 DE=-1.00D-04 OVMax= 1.88D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 3.60D-05 CP: 1.00D+00 1.36D+00 9.00D-01

E= -1276.01566450176 Delta-E= -0.000044502243 Rises=F Damp=F

DIIS: error= 7.38D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1276.01566450176 IErMin= 3 ErrMin= 5.95D-04

ErrMax= 7.38D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.00D-04 BMatP= 3.69D-04

IDIUse=3 WtCom= 2.69D-01 WtEn= 7.31D-01

Coeff-Com: -0.799D-02 0.772D-01 0.505D+00 0.426D+00

Coeff-En: 0.000D+00 0.000D+00 0.426D+00 0.574D+00

Coeff: -0.215D-02 0.208D-01 0.447D+00 0.534D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=3.09D-05 MaxDP=1.26D-03 DE=-4.45D-05 OVMax= 1.63D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.10D-05 CP: 1.00D+00 1.40D+00 1.50D+00 7.50D-01

E= -1276.01583029851 Delta-E= -0.000165796752 Rises=F Damp=F

DIIS: error= 4.04D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1276.01583029851 IErMin= 5 ErrMin= 4.04D-04

ErrMax= 4.04D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.26D-05 BMatP= 3.69D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 4.04D-03

Coeff-Com: -0.249D-02-0.467D-01 0.235D+00 0.377D+00 0.437D+00

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

Coeff: -0.248D-02-0.465D-01 0.234D+00 0.376D+00 0.440D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=1.45D-05 MaxDP=5.40D-04 DE=-1.66D-04 OVMax= 9.90D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.00D-06 CP: 1.00D+00 1.47D+00 1.63D+00 1.03D+00 9.79D-01

E= -1276.01587415858 Delta-E= -0.000043860070 Rises=F Damp=F

DIIS: error= 3.30D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1276.01587415858 IErMin= 6 ErrMin= 3.30D-04

ErrMax= 3.30D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.04D-05 BMatP= 8.26D-05

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.30D-03

Coeff-Com: 0.102D-01-0.134D+00-0.393D+00-0.234D+00-0.209D-02 0.175D+01

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

Coeff: 0.102D-01-0.133D+00-0.392D+00-0.233D+00-0.208D-02 0.175D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=5.15D-05 MaxDP=2.50D-03 DE=-4.39D-05 OVMax= 4.07D-02

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.22D-06 CP: 1.00D+00 1.69D+00 2.39D+00 1.69D+00 2.08D+00

CP: 2.78D+00

E= -1276.01595005266 Delta-E= -0.000075894086 Rises=F Damp=F

DIIS: error= 1.60D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1276.01595005266 IErMin= 7 ErrMin= 1.60D-04

ErrMax= 1.60D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.58D-06 BMatP= 1.04D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.60D-03

Coeff-Com: 0.735D-02-0.553D-01-0.392D+00-0.374D+00-0.345D+00 0.125D+01

Coeff-Com: 0.907D+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: 0.734D-02-0.552D-01-0.392D+00-0.374D+00-0.345D+00 0.125D+01

Coeff: 0.907D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=3.73D-05 MaxDP=1.80D-03 DE=-7.59D-05 OVMax= 2.90D-02

Cycle 8 Pass 1 IDiag 1:

RMSU= 6.94D-06 CP: 9.99D-01 1.85D+00 2.92D+00 2.19D+00 2.85D+00

CP: 3.00D+00 1.73D+00

E= -1276.01597383281 Delta-E= -0.000023780143 Rises=F Damp=F

DIIS: error= 5.40D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1276.01597383281 IErMin= 8 ErrMin= 5.40D-05

ErrMax= 5.40D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.72D-06 BMatP= 7.58D-06

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

Coeff-Com: -0.184D-02 0.679D-01 0.456D-01-0.286D-01-0.164D+00-0.306D+00

Coeff-Com: 0.564D+00 0.823D+00

Coeff: -0.184D-02 0.679D-01 0.456D-01-0.286D-01-0.164D+00-0.306D+00

Coeff: 0.564D+00 0.823D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=7.54D-06 MaxDP=3.96D-04 DE=-2.38D-05 OVMax= 5.56D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.33D-06 CP: 9.99D-01 1.88D+00 3.00D+00 2.29D+00 3.00D+00

CP: 3.00D+00 2.07D+00 1.19D+00

E= -1276.01597620012 Delta-E= -0.000002367313 Rises=F Damp=F

DIIS: error= 2.87D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1276.01597620012 IErMin= 9 ErrMin= 2.87D-05

ErrMax= 2.87D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.53D-07 BMatP= 2.72D-06

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

Coeff-Com: -0.207D-02 0.373D-01 0.760D-01 0.452D-01-0.246D-02-0.357D+00

Coeff-Com: 0.111D+00 0.349D+00 0.742D+00

Coeff: -0.207D-02 0.373D-01 0.760D-01 0.452D-01-0.246D-02-0.357D+00

Coeff: 0.111D+00 0.349D+00 0.742D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=2.87D-06 MaxDP=1.38D-04 DE=-2.37D-06 OVMax= 1.98D-03

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.69D-06 CP: 9.99D-01 1.89D+00 3.00D+00 2.32D+00 3.00D+00

CP: 3.00D+00 2.18D+00 1.31D+00 1.51D+00

E= -1276.01597655411 Delta-E= -0.000000353993 Rises=F Damp=F

DIIS: error= 1.60D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1276.01597655411 IErMin=10 ErrMin= 1.60D-05

ErrMax= 1.60D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.29D-07 BMatP= 4.53D-07

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

Coeff-Com: -0.367D-03-0.357D-02 0.287D-01 0.381D-01 0.633D-01-0.967D-01

Coeff-Com: -0.125D+00-0.883D-01 0.470D+00 0.714D+00

Coeff: -0.367D-03-0.357D-02 0.287D-01 0.381D-01 0.633D-01-0.967D-01

Coeff: -0.125D+00-0.883D-01 0.470D+00 0.714D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=8.37D-07 MaxDP=3.95D-05 DE=-3.54D-07 OVMax= 3.44D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 5.58D-07 CP: 9.99D-01 1.89D+00 3.00D+00 2.32D+00 3.00D+00

CP: 3.00D+00 2.20D+00 1.30D+00 1.65D+00 7.96D-01

E= -1276.01597666139 Delta-E= -0.000000107278 Rises=F Damp=F

DIIS: error= 7.07D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1276.01597666139 IErMin=11 ErrMin= 7.07D-06

ErrMax= 7.07D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.62D-08 BMatP= 2.29D-07

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

Coeff-Com: 0.271D-03-0.924D-02-0.586D-02 0.113D-02 0.155D-01 0.439D-01

Coeff-Com: -0.625D-01-0.940D-01 0.292D-01 0.315D+00 0.766D+00

Coeff: 0.271D-03-0.924D-02-0.586D-02 0.113D-02 0.155D-01 0.439D-01

Coeff: -0.625D-01-0.940D-01 0.292D-01 0.315D+00 0.766D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=5.27D-07 MaxDP=2.84D-05 DE=-1.07D-07 OVMax= 3.33D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 2.12D-07 CP: 9.99D-01 1.89D+00 3.00D+00 2.32D+00 3.00D+00

CP: 3.00D+00 2.22D+00 1.32D+00 1.74D+00 9.61D-01

CP: 1.07D+00

E= -1276.01597668606 Delta-E= -0.000000024673 Rises=F Damp=F

DIIS: error= 2.98D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1276.01597668606 IErMin=12 ErrMin= 2.98D-06

ErrMax= 2.98D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.25D-08 BMatP= 3.62D-08

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

Coeff-Com: 0.252D-03-0.475D-02-0.937D-02-0.771D-02-0.606D-02 0.499D-01

Coeff-Com: -0.130D-01-0.360D-01-0.936D-01 0.315D-01 0.447D+00 0.642D+00

Coeff: 0.252D-03-0.475D-02-0.937D-02-0.771D-02-0.606D-02 0.499D-01

Coeff: -0.130D-01-0.360D-01-0.936D-01 0.315D-01 0.447D+00 0.642D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=2.24D-07 MaxDP=1.42D-05 DE=-2.47D-08 OVMax= 1.25D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.10D-07 CP: 9.99D-01 1.89D+00 3.00D+00 2.32D+00 3.00D+00

CP: 3.00D+00 2.23D+00 1.33D+00 1.77D+00 1.02D+00

CP: 1.20D+00 1.13D+00

E= -1276.01597669354 Delta-E= -0.000000007479 Rises=F Damp=F

DIIS: error= 1.59D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1276.01597669354 IErMin=13 ErrMin= 1.59D-06

ErrMax= 1.59D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.64D-09 BMatP= 1.25D-08

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

Coeff-Com: 0.438D-04 0.382D-03-0.307D-02-0.419D-02-0.784D-02 0.121D-01

Coeff-Com: 0.982D-02 0.990D-02-0.549D-01-0.742D-01 0.487D-02 0.311D+00

Coeff-Com: 0.796D+00

Coeff: 0.438D-04 0.382D-03-0.307D-02-0.419D-02-0.784D-02 0.121D-01

Coeff: 0.982D-02 0.990D-02-0.549D-01-0.742D-01 0.487D-02 0.311D+00

Coeff: 0.796D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=2.08D-07 MaxDP=1.20D-05 DE=-7.48D-09 OVMax= 1.40D-04

Cycle 14 Pass 1 IDiag 1:

RMSU= 6.64D-08 CP: 9.99D-01 1.89D+00 3.00D+00 2.33D+00 3.00D+00

CP: 3.00D+00 2.23D+00 1.33D+00 1.81D+00 1.07D+00

CP: 1.22D+00 1.40D+00 1.24D+00

E= -1276.01597669591 Delta-E= -0.000000002364 Rises=F Damp=F

DIIS: error= 8.35D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1276.01597669591 IErMin=14 ErrMin= 8.35D-07

ErrMax= 8.35D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.03D-09 BMatP= 2.64D-09

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

Coeff-Com: -0.661D-04 0.185D-02 0.207D-02 0.111D-02-0.147D-02-0.106D-01

Coeff-Com: 0.680D-02 0.160D-01-0.298D-02-0.530D-01-0.133D+00-0.981D-02

Coeff-Com: 0.495D+00 0.689D+00

Coeff: -0.661D-04 0.185D-02 0.207D-02 0.111D-02-0.147D-02-0.106D-01

Coeff: 0.680D-02 0.160D-01-0.298D-02-0.530D-01-0.133D+00-0.981D-02

Coeff: 0.495D+00 0.689D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=5.76D-08 MaxDP=4.57D-06 DE=-2.36D-09 OVMax= 2.16D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 3.43D-08 CP: 9.99D-01 1.89D+00 3.00D+00 2.33D+00 3.00D+00

CP: 3.00D+00 2.23D+00 1.33D+00 1.81D+00 1.07D+00

CP: 1.29D+00 1.49D+00 1.39D+00 8.41D-01

E= -1276.01597669648 Delta-E= -0.000000000571 Rises=F Damp=F

DIIS: error= 3.57D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1276.01597669648 IErMin=15 ErrMin= 3.57D-07

ErrMax= 3.57D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.02D-10 BMatP= 1.03D-09

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

Coeff-Com: -0.154D-04 0.289D-03 0.388D-03 0.331D-03 0.231D-03-0.328D-02

Coeff-Com: 0.115D-02 0.307D-02 0.685D-02-0.216D-02-0.311D-01-0.550D-01

Coeff-Com: -0.258D-01 0.199D+00 0.906D+00

Coeff: -0.154D-04 0.289D-03 0.388D-03 0.331D-03 0.231D-03-0.328D-02

Coeff: 0.115D-02 0.307D-02 0.685D-02-0.216D-02-0.311D-01-0.550D-01

Coeff: -0.258D-01 0.199D+00 0.906D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=8.13D-08 MaxDP=3.75D-06 DE=-5.71D-10 OVMax= 6.13D-05

Cycle 16 Pass 1 IDiag 1:

RMSU= 1.54D-08 CP: 9.99D-01 1.89D+00 3.00D+00 2.33D+00 3.00D+00

CP: 3.00D+00 2.23D+00 1.34D+00 1.82D+00 1.10D+00

CP: 1.27D+00 1.54D+00 1.54D+00 1.11D+00 9.89D-01

E= -1276.01597669659 Delta-E= -0.000000000107 Rises=F Damp=F

DIIS: error= 2.54D-07 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1276.01597669659 IErMin=16 ErrMin= 2.54D-07

ErrMax= 2.54D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.93D-11 BMatP= 1.02D-10

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

Coeff-Com: -0.476D-05-0.120D-03 0.419D-03 0.626D-03 0.117D-02-0.169D-02

Coeff-Com: -0.181D-02-0.176D-02 0.817D-02 0.125D-01 0.398D-02-0.418D-01

Coeff-Com: -0.124D+00-0.105D-01 0.575D+00 0.579D+00

Coeff: -0.476D-05-0.120D-03 0.419D-03 0.626D-03 0.117D-02-0.169D-02

Coeff: -0.181D-02-0.176D-02 0.817D-02 0.125D-01 0.398D-02-0.418D-01

Coeff: -0.124D+00-0.105D-01 0.575D+00 0.579D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.69D-08 MaxDP=7.56D-07 DE=-1.07D-10 OVMax= 1.09D-05

Cycle 17 Pass 1 IDiag 1:

RMSU= 5.21D-09 CP: 9.99D-01 1.89D+00 3.00D+00 2.33D+00 3.00D+00

CP: 3.00D+00 2.23D+00 1.34D+00 1.82D+00 1.09D+00

CP: 1.28D+00 1.55D+00 1.55D+00 1.12D+00 1.20D+00

CP: 7.41D-01

E= -1276.01597669660 Delta-E= -0.000000000015 Rises=F Damp=F

DIIS: error= 7.79D-08 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=17 EnMin= -1276.01597669660 IErMin=17 ErrMin= 7.79D-08

ErrMax= 7.79D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.98D-12 BMatP= 5.93D-11

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

Coeff-Com: 0.299D-05-0.121D-03-0.455D-04 0.201D-04 0.192D-03 0.431D-03

Coeff-Com: -0.541D-03-0.117D-02 0.117D-02 0.468D-02 0.766D-02-0.246D-02

Coeff-Com: -0.406D-01-0.471D-01 0.327D-01 0.242D+00 0.803D+00

Coeff: 0.299D-05-0.121D-03-0.455D-04 0.201D-04 0.192D-03 0.431D-03

Coeff: -0.541D-03-0.117D-02 0.117D-02 0.468D-02 0.766D-02-0.246D-02

Coeff: -0.406D-01-0.471D-01 0.327D-01 0.242D+00 0.803D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=4.06D-09 MaxDP=2.69D-07 DE=-1.46D-11 OVMax= 1.15D-06

Error on total polarization charges = 0.06993

SCF Done: E(UB3LYP) = -1276.01597670 A.U. after 17 cycles

NFock= 17 Conv=0.41D-08 -V/T= 1.9659

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7657 S= 0.5078

<L.S>= 0.000000000000E+00

KE= 1.321006348791D+03 PE=-8.603614476662D+03 EE= 3.244635101988D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.66

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7657, after 0.7501

Leave Link 502 at Tue Sep 17 14:00:04 2019, MaxMem= 2415919104 cpu: 1734.4

(Enter /home/blab/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15337 LenP2D= 41280.

LDataN: DoStor=T MaxTD1= 6 Len= 172

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

GePol: Maximum number of non-zero 1st derivatives = 249

Leave Link 701 at Tue Sep 17 14:00:09 2019, MaxMem= 2415919104 cpu: 77.3

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 14:00:09 2019, MaxMem= 2415919104 cpu: 0.3

(Enter /home/blab/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

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

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

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

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

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Tue Sep 17 14:00:20 2019, MaxMem= 2415919104 cpu: 196.6

(Enter /home/blab/g09/l716.exe)

Dipole = 2.76223489D-13 1.26121336D-13 8.88178420D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.002545491 0.000750831 0.000000000

2 7 -0.006615591 -0.004532503 -0.000000000

3 6 0.005084313 -0.004707602 -0.000000000

4 6 0.000610930 0.004471261 0.000000000

5 6 -0.000833961 0.001472032 -0.000000000

6 7 -0.001894309 0.000862589 0.000000000

7 6 0.000595178 -0.005950718 -0.000000000

8 7 0.006767590 0.002595355 -0.000000000

9 6 -0.003012929 -0.002694575 0.000000000

10 6 0.000165367 0.001313886 0.000000000

11 6 -0.002452530 0.001825717 0.000000000

12 7 -0.004530624 -0.001905914 -0.000000000

13 6 -0.000165367 -0.001313886 -0.000000000

14 6 0.002452530 -0.001825717 0.000000000

15 6 -0.000595178 0.005950718 0.000000000

16 7 -0.006767590 -0.002595355 0.000000000

17 6 0.003012929 0.002694575 0.000000000

18 7 0.001894309 -0.000862589 -0.000000000

19 7 0.006615591 0.004532503 -0.000000000

20 6 -0.005084313 0.004707602 -0.000000000

21 6 -0.000610930 -0.004471261 -0.000000000

22 6 0.000833961 -0.001472032 0.000000000

23 6 -0.002545491 -0.000750831 -0.000000000

24 7 0.004530624 0.001905914 -0.000000000

25 30 0.000000000 -0.000000000 -0.000000000

26 6 0.001127550 -0.000404238 -0.000000000

27 1 -0.000089616 0.000422748 0.000000000

28 6 0.000021782 0.001287523 0.000000000

29 1 -0.000429430 -0.000093151 -0.000000000

30 6 -0.000021782 -0.001287523 -0.000000000

31 1 0.000429430 0.000093151 0.000000000

32 6 -0.001127550 0.000404238 0.000000000

33 1 0.000089616 -0.000422748 -0.000000000

34 1 0.000323960 0.000186850 -0.000000000

35 1 -0.000348876 -0.000082724 -0.001011495

36 1 -0.000348876 -0.000082724 0.001011495

37 1 0.000026941 -0.000482212 -0.001060597

38 1 0.000026941 -0.000482212 0.001060597

39 1 0.000078017 0.000357019 -0.000000000

40 1 -0.000026941 0.000482212 -0.001060597

41 1 -0.000026941 0.000482212 0.001060597

42 1 -0.000078017 -0.000357019 -0.000000000

43 1 0.000348876 0.000082724 -0.001011495

44 1 0.000348876 0.000082724 0.001011495

45 1 -0.000323960 -0.000186850 0.000000000

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

Cartesian Forces: Max 0.006767590 RMS 0.002092638

Leave Link 716 at Tue Sep 17 14:00:20 2019, MaxMem= 2415919104 cpu: 0.3

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

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

Internal Forces: Max 0.003224891 RMS 0.000952247

Search for a local minimum.

Step number 6 out of a maximum of 270

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

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4 5

6

DE= -1.67D-03 DEPred=-9.02D-04 R= 1.85D+00

TightC=F SS= 1.41D+00 RLast= 1.15D-01 DXNew= 5.0454D-01 3.4517D-01

Trust test= 1.85D+00 RLast= 1.15D-01 DXMaxT set to 3.45D-01

ITU= 1 1 0 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01327

Eigenvalues --- 0.01329 0.01338 0.01339 0.01606 0.01626

Eigenvalues --- 0.01635 0.01643 0.01769 0.01789 0.01803

Eigenvalues --- 0.01815 0.01885 0.01903 0.01935 0.01946

Eigenvalues --- 0.01995 0.01998 0.02044 0.02048 0.02070

Eigenvalues --- 0.02085 0.02100 0.02108 0.02112 0.02204

Eigenvalues --- 0.02312 0.02317 0.02352 0.02373 0.07193

Eigenvalues --- 0.07196 0.07196 0.07212 0.07212 0.07221

Eigenvalues --- 0.07240 0.07330 0.11074 0.13547 0.14490

Eigenvalues --- 0.14508 0.15984 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16018 0.16025

Eigenvalues --- 0.16228 0.16734 0.17423 0.22061 0.22087

Eigenvalues --- 0.22828 0.23849 0.23858 0.23961 0.24350

Eigenvalues --- 0.24994 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25041 0.25130

Eigenvalues --- 0.27348 0.30015 0.31392 0.33194 0.33203

Eigenvalues --- 0.33282 0.33282 0.33293 0.33432 0.33492

Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33727 0.33889 0.34426 0.34437

Eigenvalues --- 0.34437 0.34449 0.34504 0.35547 0.35557

Eigenvalues --- 0.35682 0.35682 0.35682 0.35802 0.38462

Eigenvalues --- 0.40928 0.41616 0.41781 0.42116 0.46309

Eigenvalues --- 0.48291 0.48942 0.48981 0.51358 0.51366

Eigenvalues --- 0.51500 0.52186 0.53261 0.53986 0.54037

Eigenvalues --- 0.55500 0.56314 0.56348 0.56837

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 0.85682 -0.02370 0.16688

Cosine: 0.997 > 0.840

Length: 0.923

GDIIS step was calculated using 3 of the last 6 vectors.

Iteration 1 RMS(Cart)= 0.00356939 RMS(Int)= 0.00000556

Iteration 2 RMS(Cart)= 0.00001019 RMS(Int)= 0.00000220

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000220

ITry= 1 IFail=0 DXMaxC= 1.63D-02 DCOld= 1.00D+10 DXMaxT= 3.45D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 5.05D-11 for atom 38.

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

(Linear) (Quad) (Total)

R1 2.59535 -0.00131 0.00398 -0.00629 -0.00231 2.59304

R2 2.71458 -0.00206 -0.00167 -0.00532 -0.00700 2.70758

R3 2.57311 0.00144 -0.00231 0.00794 0.00563 2.57874

R4 2.57101 0.00238 -0.00288 0.00740 0.00453 2.57553

R5 3.78860 0.00317 0.00339 0.00612 0.00952 3.79812

R6 2.73775 -0.00307 0.00028 -0.01072 -0.01043 2.72732

R7 2.58528 -0.00121 0.00102 0.00120 0.00221 2.58749

R8 2.62122 0.00129 -0.00035 0.00492 0.00457 2.62579

R9 2.82213 0.00059 0.00019 0.00138 0.00157 2.82370

R10 2.04608 -0.00014 0.00002 -0.00031 -0.00029 2.04578

R11 2.50544 0.00006 0.00450 -0.00786 -0.00336 2.50208

R12 2.57522 0.00258 -0.00277 0.00767 0.00491 2.58013

R13 2.78266 -0.00156 -0.00160 0.00025 -0.00135 2.78130

R14 2.60004 -0.00161 0.00368 -0.00563 -0.00195 2.59808

R15 3.77583 0.00322 0.00385 0.00505 0.00890 3.78473

R16 2.80389 -0.00174 -0.00543 0.00402 -0.00141 2.80248

R17 2.48831 0.00159 0.00052 -0.00048 0.00004 2.48835

R18 2.56609 0.00121 0.00208 -0.00218 -0.00011 2.56598

R19 2.81613 0.00035 0.00008 0.00052 0.00060 2.81672

R20 2.04501 -0.00014 0.00009 -0.00025 -0.00015 2.04486

R21 2.48831 0.00159 0.00052 -0.00048 0.00004 2.48835

R22 2.56609 0.00121 0.00208 -0.00218 -0.00011 2.56598

R23 2.80389 -0.00174 -0.00543 0.00402 -0.00141 2.80248

R24 2.81613 0.00035 0.00008 0.00052 0.00060 2.81672

R25 2.78266 -0.00156 -0.00160 0.00025 -0.00135 2.78130

R26 2.04501 -0.00014 0.00009 -0.00025 -0.00015 2.04486

R27 2.57522 0.00258 -0.00277 0.00767 0.00491 2.58013

R28 2.50544 0.00006 0.00450 -0.00786 -0.00336 2.50208

R29 2.60004 -0.00161 0.00368 -0.00563 -0.00195 2.59808

R30 3.77583 0.00322 0.00385 0.00505 0.00890 3.78473

R31 2.58528 -0.00121 0.00102 0.00120 0.00221 2.58749

R32 2.57101 0.00238 -0.00288 0.00740 0.00453 2.57553

R33 2.59535 -0.00131 0.00398 -0.00629 -0.00231 2.59304

R34 3.78860 0.00317 0.00339 0.00612 0.00952 3.79812

R35 2.73775 -0.00307 0.00028 -0.01072 -0.01043 2.72732

R36 2.62122 0.00129 -0.00035 0.00492 0.00457 2.62579

R37 2.82213 0.00059 0.00019 0.00138 0.00157 2.82370

R38 2.71458 -0.00206 -0.00167 -0.00532 -0.00700 2.70758

R39 2.04608 -0.00014 0.00002 -0.00031 -0.00029 2.04578

R40 2.57311 0.00144 -0.00231 0.00794 0.00563 2.57874

R41 2.06560 -0.00037 -0.00012 -0.00068 -0.00081 2.06479

R42 2.07317 -0.00098 -0.00075 -0.00173 -0.00248 2.07069

R43 2.07317 -0.00098 -0.00075 -0.00173 -0.00248 2.07069

R44 2.07234 -0.00111 -0.00095 -0.00180 -0.00275 2.06959

R45 2.07234 -0.00111 -0.00095 -0.00180 -0.00275 2.06959

R46 2.06373 -0.00024 -0.00018 -0.00043 -0.00061 2.06311

R47 2.07234 -0.00111 -0.00095 -0.00180 -0.00275 2.06959

R48 2.07234 -0.00111 -0.00095 -0.00180 -0.00275 2.06959

R49 2.06373 -0.00024 -0.00018 -0.00043 -0.00061 2.06311

R50 2.07317 -0.00098 -0.00075 -0.00173 -0.00248 2.07069

R51 2.07317 -0.00098 -0.00075 -0.00173 -0.00248 2.07069

R52 2.06560 -0.00037 -0.00012 -0.00068 -0.00081 2.06479

A1 1.89180 -0.00113 -0.00219 -0.00077 -0.00297 1.88884

A2 2.19762 0.00181 -0.00013 0.00438 0.00426 2.20188

A3 2.19376 -0.00068 0.00231 -0.00361 -0.00129 2.19246

A4 1.89620 0.00210 0.00191 0.00316 0.00506 1.90127

A5 2.18737 -0.00024 -0.00122 0.00060 -0.00062 2.18675

A6 2.19961 -0.00185 -0.00069 -0.00376 -0.00444 2.19517

A7 1.90878 -0.00257 -0.00146 -0.00441 -0.00586 1.90292

A8 2.21273 0.00127 0.00235 -0.00064 0.00170 2.21443

A9 2.16167 0.00130 -0.00089 0.00505 0.00416 2.16583

A10 1.84735 0.00149 0.00107 0.00285 0.00392 1.85128

A11 2.19226 -0.00145 -0.00205 -0.00015 -0.00220 2.19006

A12 2.24357 -0.00004 0.00098 -0.00270 -0.00172 2.24185

A13 1.88063 0.00011 0.00067 -0.00083 -0.00016 1.88047

A14 2.18716 -0.00047 -0.00059 -0.00024 -0.00082 2.18633

A15 2.21540 0.00036 -0.00009 0.00106 0.00098 2.21638

A16 2.16317 0.00073 -0.00169 0.00382 0.00212 2.16529

A17 2.22969 0.00045 0.00006 0.00242 0.00247 2.23216

A18 2.16313 0.00184 -0.00010 0.00475 0.00464 2.16777

A19 1.89036 -0.00229 0.00005 -0.00717 -0.00711 1.88325

A20 1.90605 0.00139 0.00017 0.00503 0.00520 1.91125

A21 2.20124 -0.00149 0.00048 -0.00461 -0.00413 2.19711

A22 2.17589 0.00010 -0.00065 -0.00042 -0.00107 2.17483

A23 1.88608 -0.00009 -0.00059 -0.00168 -0.00227 1.88381

A24 2.23046 0.00152 -0.00143 0.00755 0.00612 2.23658

A25 2.16665 -0.00143 0.00202 -0.00587 -0.00385 2.16280

A26 1.86116 -0.00029 0.00069 -0.00098 -0.00030 1.86086

A27 2.16953 -0.00080 0.00118 -0.00486 -0.00368 2.16585

A28 2.25250 0.00109 -0.00187 0.00584 0.00398 2.25647

A29 1.88112 0.00128 -0.00031 0.00479 0.00449 1.88561

A30 2.17623 -0.00106 0.00082 -0.00561 -0.00480 2.17143

A31 2.22583 -0.00022 -0.00051 0.00082 0.00031 2.22614

A32 2.19337 -0.00230 0.00291 -0.00933 -0.00642 2.18695

A33 1.86116 -0.00029 0.00069 -0.00098 -0.00030 1.86086

A34 2.25250 0.00109 -0.00187 0.00584 0.00398 2.25647

A35 2.16953 -0.00080 0.00118 -0.00486 -0.00368 2.16585

A36 1.88112 0.00128 -0.00031 0.00479 0.00449 1.88561

A37 2.22583 -0.00022 -0.00051 0.00082 0.00031 2.22614

A38 2.17623 -0.00106 0.00082 -0.00561 -0.00480 2.17143

A39 1.89036 -0.00229 0.00005 -0.00717 -0.00711 1.88325

A40 2.16313 0.00184 -0.00010 0.00475 0.00464 2.16777

A41 2.22969 0.00045 0.00006 0.00242 0.00247 2.23216

A42 1.90605 0.00139 0.00017 0.00503 0.00520 1.91125

A43 2.20124 -0.00149 0.00048 -0.00461 -0.00413 2.19711

A44 2.17589 0.00010 -0.00065 -0.00042 -0.00107 2.17483

A45 2.16665 -0.00143 0.00202 -0.00587 -0.00385 2.16280

A46 2.23046 0.00152 -0.00143 0.00755 0.00612 2.23658

A47 1.88608 -0.00009 -0.00059 -0.00168 -0.00227 1.88381

A48 2.16317 0.00073 -0.00169 0.00382 0.00212 2.16529

A49 1.89620 0.00210 0.00191 0.00316 0.00506 1.90127

A50 2.19961 -0.00185 -0.00069 -0.00376 -0.00444 2.19517

A51 2.18737 -0.00024 -0.00122 0.00060 -0.00062 2.18675

A52 2.21273 0.00127 0.00235 -0.00064 0.00170 2.21443

A53 2.16167 0.00130 -0.00089 0.00505 0.00416 2.16583

A54 1.90878 -0.00257 -0.00146 -0.00441 -0.00586 1.90292

A55 1.84735 0.00149 0.00107 0.00285 0.00392 1.85128

A56 2.19226 -0.00145 -0.00205 -0.00015 -0.00220 2.19006

A57 2.24357 -0.00004 0.00098 -0.00270 -0.00172 2.24185

A58 1.88063 0.00011 0.00067 -0.00083 -0.00016 1.88047

A59 2.21540 0.00036 -0.00009 0.00106 0.00098 2.21638

A60 2.18716 -0.00047 -0.00059 -0.00024 -0.00082 2.18633

A61 1.89180 -0.00113 -0.00219 -0.00077 -0.00297 1.88884

A62 2.19762 0.00181 -0.00013 0.00438 0.00426 2.20188

A63 2.19376 -0.00068 0.00231 -0.00361 -0.00129 2.19246

A64 2.19337 -0.00230 0.00291 -0.00933 -0.00642 2.18695

A65 1.55993 0.00089 -0.00051 0.00278 0.00228 1.56221

A66 1.58166 -0.00089 0.00051 -0.00278 -0.00228 1.57938

A67 1.58166 -0.00089 0.00051 -0.00278 -0.00228 1.57938

A68 1.55993 0.00089 -0.00051 0.00278 0.00228 1.56221

A69 1.94154 -0.00005 0.00121 -0.00085 0.00036 1.94191

A70 1.94751 0.00041 0.00075 0.00164 0.00240 1.94991

A71 1.94751 0.00041 0.00075 0.00164 0.00240 1.94991

A72 1.88149 -0.00015 -0.00055 -0.00064 -0.00119 1.88030

A73 1.88149 -0.00015 -0.00055 -0.00064 -0.00119 1.88030

A74 1.86049 -0.00052 -0.00184 -0.00130 -0.00314 1.85735

A75 1.93874 0.00028 0.00080 0.00038 0.00118 1.93992

A76 1.93874 0.00028 0.00080 0.00038 0.00118 1.93992

A77 1.94226 0.00031 0.00081 0.00145 0.00226 1.94452

A78 1.86054 -0.00041 -0.00119 -0.00183 -0.00302 1.85751

A79 1.89034 -0.00026 -0.00069 -0.00027 -0.00096 1.88938

A80 1.89034 -0.00026 -0.00069 -0.00027 -0.00096 1.88938

A81 1.93874 0.00028 0.00080 0.00038 0.00118 1.93992

A82 1.93874 0.00028 0.00080 0.00038 0.00118 1.93992

A83 1.94226 0.00031 0.00081 0.00145 0.00226 1.94452

A84 1.86054 -0.00041 -0.00119 -0.00183 -0.00302 1.85751

A85 1.89034 -0.00026 -0.00069 -0.00027 -0.00096 1.88938

A86 1.89034 -0.00026 -0.00069 -0.00027 -0.00096 1.88938

A87 1.94751 0.00041 0.00075 0.00164 0.00240 1.94991

A88 1.94751 0.00041 0.00075 0.00164 0.00240 1.94991

A89 1.94154 -0.00005 0.00121 -0.00085 0.00036 1.94191

A90 1.86049 -0.00052 -0.00184 -0.00130 -0.00314 1.85735

A91 1.88149 -0.00015 -0.00055 -0.00064 -0.00119 1.88030

A92 1.88149 -0.00015 -0.00055 -0.00064 -0.00119 1.88030

A93 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

A94 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

A95 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

A96 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D1 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D2 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D3 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D4 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D6 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D7 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D10 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D11 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D12 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D13 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D14 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D15 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D16 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D17 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D18 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D19 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D20 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D21 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D22 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D23 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D24 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D25 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D26 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D27 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D28 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D29 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D30 1.03965 -0.00005 -0.00066 0.00028 -0.00038 1.03928

D31 -1.03965 0.00005 0.00066 -0.00028 0.00038 -1.03928

D32 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.10194 -0.00005 -0.00066 0.00028 -0.00038 -2.10232

D34 2.10194 0.00005 0.00066 -0.00028 0.00038 2.10232

D35 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D36 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D37 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D38 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D39 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D40 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D41 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D42 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D43 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D44 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D45 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D46 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D47 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D48 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D49 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D50 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D51 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D52 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D53 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D54 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D55 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D56 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D57 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D58 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D59 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D60 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D61 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D62 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D63 1.03389 -0.00008 -0.00023 -0.00090 -0.00113 1.03276

D64 -1.03389 0.00008 0.00023 0.00090 0.00113 -1.03276

D65 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D66 -2.10770 -0.00008 -0.00023 -0.00090 -0.00113 -2.10883

D67 2.10770 0.00008 0.00023 0.00090 0.00113 2.10883

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D70 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D71 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D72 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D73 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D74 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D75 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D76 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D77 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D78 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D79 -2.10770 -0.00008 -0.00023 -0.00090 -0.00113 -2.10883

D80 2.10770 0.00008 0.00023 0.00090 0.00113 2.10883

D81 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D82 1.03389 -0.00008 -0.00023 -0.00090 -0.00113 1.03276

D83 -1.03389 0.00008 0.00023 0.00090 0.00113 -1.03276

D84 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D85 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D86 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D87 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D88 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D89 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D90 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D91 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D92 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D93 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D94 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D95 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D96 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D97 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D98 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D99 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D100 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D101 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D102 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D103 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D104 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D105 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D106 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D107 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D108 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D109 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D110 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D111 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D112 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D113 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D114 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D116 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D117 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D118 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D119 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D120 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D121 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D122 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D123 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D124 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D125 1.03965 -0.00005 -0.00066 0.00028 -0.00038 1.03928

D126 -1.03965 0.00005 0.00066 -0.00028 0.00038 -1.03928

D127 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D128 -2.10194 -0.00005 -0.00066 0.00028 -0.00038 -2.10232

D129 2.10194 0.00005 0.00066 -0.00028 0.00038 2.10232

D130 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D131 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D132 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D133 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D134 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D135 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D136 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

Item Value Threshold Converged?

Maximum Force 0.003225 0.000450 NO

RMS Force 0.000952 0.000300 NO

Maximum Displacement 0.016313 0.001800 NO

RMS Displacement 0.003568 0.001200 NO

Predicted change in Energy=-3.507272D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:00:20 2019, MaxMem= 2415919104 cpu: 1.8

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

Input orientation:

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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1 6 0 -2.071281 -2.195216 -0.000000

2 7 0 -0.738361 -1.869338 -0.000000

3 6 0 -0.002603 -3.016593 -0.000000

4 6 0 -0.897048 -4.149245 -0.000000

5 6 0 -2.183300 -3.623618 -0.000000

6 7 0 1.362955 -3.116987 -0.000000

7 6 0 2.182964 -2.077432 -0.000000

8 7 0 1.856364 -0.751726 -0.000000

9 6 0 3.004861 0.004024 -0.000000

10 6 0 4.161929 -0.923610 -0.000000

11 6 0 3.651068 -2.181704 -0.000000

12 7 0 -3.115051 -1.316184 -0.000000

13 6 0 -4.161929 0.923610 -0.000000

14 6 0 -3.651068 2.181704 -0.000000

15 6 0 -2.182964 2.077432 -0.000000

16 7 0 -1.856364 0.751726 -0.000000

17 6 0 -3.004861 -0.004024 -0.000000

18 7 0 -1.362955 3.116987 -0.000000

19 7 0 0.738361 1.869338 -0.000000

20 6 0 0.002603 3.016593 -0.000000

21 6 0 0.897048 4.149245 -0.000000

22 6 0 2.183300 3.623618 -0.000000

23 6 0 2.071281 2.195216 -0.000000

24 7 0 3.115051 1.316184 -0.000000

25 30 0 0.000000 -0.000000 -0.000000

26 6 0 -0.479642 -5.584001 -0.000000

27 1 0 -3.113354 -4.177679 -0.000000

28 6 0 5.585921 -0.483184 -0.000000

29 1 0 4.197851 -3.115487 -0.000000

30 6 0 -5.585921 0.483184 -0.000000

31 1 0 -4.197851 3.115487 -0.000000

32 6 0 0.479642 5.584001 -0.000000

33 1 0 3.113354 4.177679 -0.000000

34 1 0 -1.346678 -6.248917 -0.000000

35 1 0 0.129048 -5.829269 0.877516

36 1 0 0.129048 -5.829269 -0.877516

37 1 0 5.808755 0.133624 0.877104

38 1 0 5.808755 0.133624 -0.877104

39 1 0 6.267029 -1.336423 -0.000000

40 1 0 -5.808755 -0.133624 0.877104

41 1 0 -5.808755 -0.133624 -0.877104

42 1 0 -6.267029 1.336423 -0.000000

43 1 0 -0.129048 5.829269 0.877516

44 1 0 -0.129048 5.829269 -0.877516

45 1 0 1.346678 6.248917 -0.000000

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Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.372177 0.000000

3 C 2.225778 1.362914 0.000000

4 C 2.279705 2.285423 1.443237 0.000000

5 C 1.432788 2.272739 2.263608 1.389507 0.000000

6 N 3.555789 2.443800 1.369243 2.484586 3.582261

7 C 4.255875 2.928728 2.378808 3.711992 4.631949

8 N 4.184502 2.825183 2.930082 4.373147 4.956476

9 C 5.532076 4.185833 4.262506 5.698643 6.330624

10 C 6.361594 4.990716 4.660891 5.999831 6.895794

11 C 5.722365 4.400530 3.747846 4.955460 6.009906

12 N 1.364608 2.440212 3.546650 3.598024 2.488456

13 C 3.754715 4.418300 5.729327 6.032687 4.959058

14 C 4.653295 4.989469 6.350873 6.904024 5.987997

15 C 4.274108 4.202841 5.541035 6.358073 5.701050

16 N 2.954768 2.849546 4.199602 4.993978 4.387542

17 C 2.381784 2.935374 4.253131 4.650348 3.711661

18 N 5.359219 5.025292 6.282624 7.281154 6.790341

19 N 4.941122 4.019753 4.941797 6.236819 6.221630

20 C 5.609273 4.941797 6.033188 7.222092 6.990749

21 C 7.004510 6.236819 7.222092 8.490214 8.360978

22 C 7.208348 6.221630 6.990749 8.360978 8.461065

23 C 6.036282 4.941122 5.609273 7.004510 7.208348

24 N 6.263223 4.999634 5.337857 6.779960 7.243905

25 Zn 3.018141 2.009877 3.016594 4.245107 4.230533

26 C 3.743952 3.723661 2.611350 1.494239 2.597220

27 H 2.239659 3.311951 3.320375 2.216488 1.082581

28 C 7.846259 6.474409 6.135940 7.447744 8.379923

29 H 6.336317 5.091079 4.201618 5.198716 6.401351

30 C 4.418882 5.388246 6.589528 6.591277 5.333259

31 H 5.720653 6.067665 7.429840 7.979452 7.033773

32 C 8.186783 7.552205 8.614103 9.830125 9.584963

33 H 8.215486 7.169527 7.840072 9.242347 9.429463

34 H 4.117954 4.421624 3.500637 2.147275 2.755382

35 H 4.337952 4.147708 2.949324 2.155316 3.313893

36 H 4.337952 4.147708 2.949324 2.155316 3.313893

37 H 8.263641 6.902601 6.668213 8.005003 8.874634

38 H 8.263641 6.902601 6.668213 8.005003 8.874634

39 H 8.382418 7.025631 6.490859 7.696491 8.754389

40 H 4.357543 5.430553 6.541576 6.404638 5.108159

41 H 4.357543 5.430553 6.541576 6.404638 5.108159

42 H 5.484230 6.390859 7.628354 7.676540 6.424862

43 H 8.302690 7.772378 8.890180 10.046423 9.713241

44 H 8.302690 7.772378 8.890180 10.046423 9.713241

45 H 9.109656 8.381734 9.363239 10.637485 10.484641

6 7 8 9 10

6 N 0.000000

7 C 1.324043 0.000000

8 N 2.416177 1.365344 0.000000

9 C 3.526551 2.237850 1.374846 0.000000

10 C 3.556004 2.290766 2.311963 1.483007 0.000000

11 C 2.471886 1.471802 2.294733 2.279252 1.357858

12 N 4.826534 5.352426 5.003357 6.260692 7.287561

13 C 6.844762 7.018826 6.247128 7.225546 8.526361

14 C 7.294968 7.223307 6.239938 7.003119 8.407490

15 C 6.289319 6.026958 4.931563 5.586819 7.018826

16 N 5.032987 4.931563 4.005586 4.918391 6.247128

17 C 5.363614 5.586819 4.918391 6.009727 7.225546

18 N 6.803898 6.289319 5.032987 5.363614 6.844762

19 N 5.025292 4.202841 2.849546 2.935374 4.418300

20 C 6.282624 5.541035 4.199602 4.253131 5.729327

21 C 7.281154 6.358073 4.993978 4.650348 6.032687

22 C 6.790341 5.701050 4.387542 3.711661 4.959058

23 C 5.359219 4.274108 2.954768 2.381784 3.754715

24 N 4.766849 3.519292 2.420856 1.316779 2.472373

25 Zn 3.401949 3.013479 2.002793 3.004863 4.263180

26 C 3.079175 4.402896 5.367290 6.585422 6.577494

27 H 4.600261 5.697545 6.036161 7.410748 7.969862

28 C 4.976983 3.757890 3.739212 2.626641 1.490546

29 H 2.834897 2.266568 3.327150 3.339847 2.192172

30 C 7.826117 8.179995 7.544044 8.604134 9.848839

31 H 8.352623 8.226860 7.183931 7.846035 9.284408

32 C 8.745710 7.848494 6.483579 6.124776 7.477181

33 H 7.501736 6.323926 5.087146 4.175065 5.207941

34 H 4.141388 5.464399 6.362279 7.618081 7.661831

35 H 3.106289 4.366335 5.434620 6.562594 6.410901

36 H 3.106289 4.366335 5.434620 6.562594 6.410901

37 H 5.576821 4.336409 4.144219 2.940736 2.144549

38 H 5.576821 4.336409 4.144219 2.940736 2.144549

39 H 5.217313 4.150745 4.449251 3.526831 2.145195

40 H 7.816852 8.271352 7.739859 8.858221 10.040315

41 H 7.816852 8.271352 7.739859 8.858221 10.040315

42 H 8.834564 9.113550 8.387484 9.367136 10.671032

43 H 9.112168 8.284405 6.929747 6.672699 8.048844

44 H 9.112168 8.284405 6.929747 6.672699 8.048844

45 H 9.365919 8.368242 7.019173 6.461290 7.705244

11 12 13 14 15

11 C 0.000000

12 N 6.821253 0.000000

13 C 8.407490 2.472373 0.000000

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16 N 6.239938 2.420856 2.311963 2.294733 1.365344

17 C 7.003119 1.316779 1.483007 2.279252 2.237850

18 N 7.294968 4.766849 3.556004 2.471886 1.324043

19 N 4.989469 4.999634 4.990716 4.400530 2.928728

20 C 6.350873 5.337857 4.660891 3.747846 2.378808

21 C 6.904024 6.779960 5.999831 4.955460 3.711992

22 C 5.987997 7.243905 6.895794 6.009906 4.631949

23 C 4.653295 6.263223 6.361594 5.722365 4.255875

24 N 3.538719 6.763396 7.287561 6.821253 5.352426

25 Zn 4.253249 3.381698 4.263180 4.253249 3.013479

26 C 5.351485 5.015939 7.477181 8.388332 7.848494

27 H 7.052753 2.861495 5.207941 6.382075 6.323926

28 C 2.574611 8.740755 9.848839 9.613719 8.179995

29 H 1.082092 7.531005 9.284408 9.469201 8.226860

30 C 9.613719 3.056619 1.490546 2.574611 3.757890

31 H 9.469201 4.562035 2.192172 1.082092 2.266568

32 C 8.388332 7.780383 6.577494 5.351485 4.402896

33 H 6.382075 8.305152 7.969862 7.052753 5.697545

34 H 6.443578 5.240134 7.705244 8.739884 8.368242

35 H 5.145813 5.626914 8.048844 8.901404 8.284405

36 H 5.145813 5.626914 8.048844 8.901404 8.284405

37 H 3.284154 9.083257 10.040315 9.718652 8.271352

38 H 3.284154 9.083257 10.040315 9.718652 8.271352

39 H 2.749136 9.382102 10.671032 10.523586 9.113550

40 H 9.718652 3.069820 2.144549 3.284154 4.336409

41 H 9.718652 3.069820 2.144549 3.284154 4.336409

42 H 10.523586 4.119622 2.145195 2.749136 4.150745

43 H 8.901404 7.793827 6.410901 5.145813 4.366335

44 H 8.901404 7.793827 6.410901 5.145813 4.366335

45 H 8.739884 8.782811 7.661831 6.443578 5.464399

16 17 18 19 20

16 N 0.000000

17 C 1.374846 0.000000

18 N 2.416177 3.526551 0.000000

19 N 2.825183 4.185833 2.443800 0.000000

20 C 2.930082 4.262506 1.369243 1.362914 0.000000

21 C 4.373147 5.698643 2.484586 2.285423 1.443237

22 C 4.956476 6.330624 3.582261 2.272739 2.263608

23 C 4.184502 5.532076 3.555789 1.372177 2.225778

24 N 5.003357 6.260692 4.826534 2.440212 3.546650

25 Zn 2.002793 3.004863 3.401949 2.009877 3.016594

26 C 6.483579 6.124776 8.745710 7.552205 8.614103

27 H 5.087146 4.175065 7.501736 7.169527 7.840072

28 C 7.544044 8.604134 7.826117 5.388246 6.589528

29 H 7.183931 7.846035 8.352623 6.067665 7.429840

30 C 3.739212 2.626641 4.976983 6.474409 6.135940

31 H 3.327150 3.339847 2.834897 5.091079 4.201618

32 C 5.367290 6.585422 3.079175 3.723661 2.611350

33 H 6.036161 7.410748 4.600261 3.311951 3.320375

34 H 7.019173 6.461290 9.365919 8.381734 9.363239

35 H 6.929747 6.672699 9.112168 7.772378 8.890180

36 H 6.929747 6.672699 9.112168 7.772378 8.890180

37 H 7.739859 8.858221 7.816852 5.430553 6.541576

38 H 7.739859 8.858221 7.816852 5.430553 6.541576

39 H 8.387484 9.367136 8.834564 6.390859 7.628354

40 H 4.144219 2.940736 5.576821 6.902601 6.668213

41 H 4.144219 2.940736 5.576821 6.902601 6.668213

42 H 4.449251 3.526831 5.217313 7.025631 6.490859

43 H 5.434620 6.562594 3.106289 4.147708 2.949324

44 H 5.434620 6.562594 3.106289 4.147708 2.949324

45 H 6.362279 7.618081 4.141388 4.421624 3.500637

21 22 23 24 25

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22 C 1.389507 0.000000

23 C 2.279705 1.432788 0.000000

24 N 3.598024 2.488456 1.364608 0.000000

25 Zn 4.245107 4.230533 3.018141 3.381698 0.000000

26 C 9.830125 9.584963 8.186783 7.780383 5.604563

27 H 9.242347 9.429463 8.215486 8.305152 5.210179

28 C 6.591277 5.333259 4.418882 3.056619 5.606779

29 H 7.979452 7.033773 5.720653 4.562035 5.227640

30 C 7.447744 8.379923 7.846259 8.740755 5.606779

31 H 5.198716 6.401351 6.336317 7.531005 5.227640

32 C 1.494239 2.597220 3.743952 5.015939 5.604563

33 H 2.216488 1.082581 2.239659 2.861495 5.210179

34 H 10.637485 10.484641 9.109656 8.782811 6.392379

35 H 10.046423 9.713241 8.302690 7.793827 5.896360

36 H 10.046423 9.713241 8.302690 7.793827 5.896360

37 H 6.404638 5.108159 4.357543 3.069820 5.876121

38 H 6.404638 5.108159 4.357543 3.069820 5.876121

39 H 7.676540 6.424862 5.484230 4.119622 6.407939

40 H 8.005003 8.874634 8.263641 9.083257 5.876121

41 H 8.005003 8.874634 8.263641 9.083257 5.876121

42 H 7.696491 8.754389 8.382418 9.382102 6.407939

43 H 2.155316 3.313893 4.337952 5.626914 5.896360

44 H 2.155316 3.313893 4.337952 5.626914 5.896360

45 H 2.147275 2.755382 4.117954 5.240134 6.392379

26 27 28 29 30

26 C 0.000000

27 H 2.985662 0.000000

28 C 7.925237 9.451278 0.000000

29 H 5.288904 7.387961 2.975862 0.000000

30 C 7.929995 5.276100 11.213559 10.424617 0.000000

31 H 9.460770 7.373358 10.424617 10.455280 2.975862

32 C 11.209126 10.401923 7.929995 9.460770 7.925237

33 H 10.401923 10.420359 5.276100 7.373358 9.451278

34 H 1.092641 2.722347 9.016906 6.368688 7.955650

35 H 1.095763 3.743121 7.689481 4.968884 8.560255

36 H 1.095763 3.743121 7.689481 4.968884 8.560255

37 H 8.544267 9.947897 1.095180 3.731092 11.433728

38 H 8.544267 9.947897 1.095180 3.731092 11.433728

39 H 7.972421 9.801240 1.091753 2.728840 11.991805

40 H 7.673028 4.938509 11.433728 10.478215 1.095180

41 H 7.673028 4.938509 11.433728 10.478215 1.095180

42 H 9.021425 6.352243 11.991805 11.372477 1.091753

43 H 11.452322 10.479271 8.560255 9.975007 7.689481

44 H 11.452322 10.479271 8.560255 9.975007 7.689481

45 H 11.973028 11.340449 7.955650 9.788834 9.016906

31 32 33 34 35

31 H 0.000000

32 C 5.288904 0.000000

33 H 7.387961 2.985662 0.000000

34 H 9.788834 11.973028 11.340449 0.000000

35 H 9.975007 11.452322 10.479271 1.767458 0.000000

36 H 9.975007 11.452322 10.479271 1.767458 1.755033

37 H 10.478215 7.673028 4.938509 9.628415 8.234996

38 H 10.478215 7.673028 4.938509 9.628415 8.419849

39 H 11.372477 9.021425 6.352243 9.060968 7.657056

40 H 3.731092 8.544267 9.947897 7.620777 8.227872

41 H 3.731092 8.544267 9.947897 7.620777 8.412881

42 H 2.728840 7.972421 9.801240 9.041418 9.645050

43 H 4.968884 1.095763 3.743121 12.171082 11.661395

44 H 4.968884 1.095763 3.743121 12.171082 11.792721

45 H 6.368688 1.092641 2.722347 12.784758 12.171082

36 37 38 39 40

36 H 0.000000

37 H 8.419849 0.000000

38 H 8.234996 1.754208 0.000000

39 H 7.657056 1.772108 1.772108 0.000000

40 H 8.412881 11.620583 11.752242 12.167193 0.000000

41 H 8.227872 11.752242 11.620583 12.167193 1.754208

42 H 9.645050 12.167193 12.167193 12.815878 1.772108

43 H 11.792721 8.227872 8.412881 9.645050 8.234996

44 H 11.661395 8.412881 8.227872 9.645050 8.419849

45 H 12.171082 7.620777 7.620777 9.041418 9.628415

41 42 43 44 45

41 H 0.000000

42 H 1.772108 0.000000

43 H 8.419849 7.657056 0.000000

44 H 8.234996 7.657056 1.755033 0.000000

45 H 9.628415 9.060968 1.767458 1.767458 0.000000

Stoichiometry C20H16N8Zn(1-,2)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=3 Diff= 5.59D-01

Largest Abelian subgroup C2H NOp 4

Largest concise Abelian subgroup C2H 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 -3.018114 -0.012903 0.000000

2 7 0 -1.863160 -0.753816 0.000000

3 6 0 -2.187014 -2.077693 0.000000

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5 6 0 -4.130072 -0.916468 0.000000

6 7 0 -1.318352 -3.136113 0.000000

7 6 0 0.000000 -3.013479 0.000000

8 7 0 0.735190 -1.862975 0.000000

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10 6 0 2.200088 -3.651619 0.000000

11 6 0 0.936547 -4.148856 0.000000

12 7 0 -3.100897 1.349192 0.000000

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17 6 0 -2.074406 2.173947 0.000000

18 7 0 1.318352 3.136113 0.000000

19 7 0 1.863160 0.753816 0.000000

20 6 0 2.187014 2.077693 0.000000

21 6 0 3.624120 2.210586 0.000000

22 6 0 4.130072 0.916468 0.000000

23 6 0 3.018114 0.012903 0.000000

24 7 0 3.100897 -1.349192 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -4.375706 -3.502046 0.000000

27 1 0 -5.172594 -0.624695 0.000000

28 6 0 3.500803 -4.379538 0.000000

29 1 0 0.637056 -5.188678 0.000000

30 6 0 -3.500803 4.379538 0.000000

31 1 0 -0.637056 5.188678 0.000000

32 6 0 4.375706 3.502046 0.000000

33 1 0 5.172594 0.624695 0.000000

34 1 0 -5.455088 -3.332345 0.000000

35 1 0 -4.133759 -4.112064 0.877516

36 1 0 -4.133759 -4.112064 -0.877516

37 1 0 4.101237 -4.115743 0.877104

38 1 0 4.101237 -4.115743 -0.877104

39 1 0 3.352260 -5.461139 0.000000

40 1 0 -4.101237 4.115743 0.877104

41 1 0 -4.101237 4.115743 -0.877104

42 1 0 -3.352260 5.461139 0.000000

43 1 0 4.133759 4.112064 0.877516

44 1 0 4.133759 4.112064 -0.877516

45 1 0 5.455088 3.332345 0.000000

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

Rotational constants (GHZ): 0.1829358 0.1817816 0.0913831

Leave Link 202 at Tue Sep 17 14:00:20 2019, MaxMem= 2415919104 cpu: 0.2

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 229 symmetry adapted cartesian basis functions of AG symmetry.

There are 82 symmetry adapted cartesian basis functions of BG symmetry.

There are 78 symmetry adapted cartesian basis functions of AU symmetry.

There are 218 symmetry adapted cartesian basis functions of BU symmetry.

There are 212 symmetry adapted basis functions of AG symmetry.

There are 82 symmetry adapted basis functions of BG symmetry.

There are 78 symmetry adapted basis functions of AU symmetry.

There are 204 symmetry adapted basis functions of BU symmetry.

576 basis functions, 1015 primitive gaussians, 607 cartesian basis functions

103 alpha electrons 102 beta electrons

nuclear repulsion energy 2761.1613542539 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= 45 NActive= 45 NUniq= 21 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1141806397 Hartrees.

Nuclear repulsion after empirical dispersion term = 2761.0471736142 Hartrees.

No density basis found on file 724.

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

Polarizable Continuum Model (PCM)

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

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

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 = 45

GePol: Total number of spheres = 45

GePol: Number of exposed spheres = 45 (100.00%)

GePol: Number of points = 3518

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.17D-08

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 192

GePol: Fraction of low-weight points (<1% of avg) = 5.46%

GePol: Cavity surface area = 381.678 Ang\*\*2

GePol: Cavity volume = 380.804 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0106222491 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2761.0365513651 Hartrees.

Leave Link 301 at Tue Sep 17 14:00:20 2019, MaxMem= 2415919104 cpu: 2.1

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15325 LenP2D= 41250.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.78D-04 NBF= 212 82 78 204

NBsUse= 576 1.00D-06 EigRej= -1.00D+00 NBFU= 212 82 78 204

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= 594 594 594 594 594 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Tue Sep 17 14:00:21 2019, MaxMem= 2415919104 cpu: 13.0

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:00:21 2019, MaxMem= 2415919104 cpu: 1.5

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

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

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.980264 0.000000 0.000000 0.197693 Ang= 22.80 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-BG.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7657 S= 0.5078

Leave Link 401 at Tue Sep 17 14:00:22 2019, MaxMem= 2415919104 cpu: 21.2

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1141655 IEndB= 1141655 NGot= 2415919104 MDV= 2415163146

LenX= 2415163146 LenY= 2414794090

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= 670000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 37128972.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.55D-15 for 3515.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.47D-15 for 3504 2634.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.44D-15 for 3515.

Iteration 1 A^-1\*A deviation from orthogonality is 1.31D-12 for 1457 1438.

E= -1276.01718952708

DIIS: error= 4.83D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1276.01718952708 IErMin= 1 ErrMin= 4.83D-04

ErrMax= 4.83D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.90D-04 BMatP= 4.90D-04

IDIUse=3 WtCom= 9.95D-01 WtEn= 4.83D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.295 Goal= None Shift= 0.000

Gap= 0.343 Goal= None Shift= 0.000

RMSDP=3.50D-05 MaxDP=1.41D-03 OVMax= 6.87D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.50D-05 CP: 1.00D+00

E= -1276.01731015062 Delta-E= -0.000120623539 Rises=F Damp=F

DIIS: error= 2.33D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1276.01731015062 IErMin= 2 ErrMin= 2.33D-04

ErrMax= 2.33D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.54D-05 BMatP= 4.90D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.33D-03

Coeff-Com: 0.181D+00 0.819D+00

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

Coeff: 0.181D+00 0.819D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=1.61D-05 MaxDP=6.19D-04 DE=-1.21D-04 OVMax= 5.76D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.61D-05 CP: 1.00D+00 9.67D-01

E= -1276.01729855714 Delta-E= 0.000011593483 Rises=F Damp=F

DIIS: error= 3.30D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1276.01731015062 IErMin= 2 ErrMin= 2.33D-04

ErrMax= 3.30D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.52D-04 BMatP= 8.54D-05

IDIUse=3 WtCom= 3.55D-01 WtEn= 6.45D-01

Coeff-Com: -0.630D-02 0.577D+00 0.429D+00

Coeff-En: 0.000D+00 0.593D+00 0.407D+00

Coeff: -0.224D-02 0.587D+00 0.415D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=9.10D-06 MaxDP=3.83D-04 DE= 1.16D-05 OVMax= 1.57D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 5.05D-06 CP: 1.00D+00 1.05D+00 5.69D-01

E= -1276.01733206647 Delta-E= -0.000033509329 Rises=F Damp=F

DIIS: error= 6.94D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1276.01733206647 IErMin= 4 ErrMin= 6.94D-05

ErrMax= 6.94D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.79D-06 BMatP= 8.54D-05

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

Coeff-Com: -0.916D-02 0.207D+00 0.153D+00 0.649D+00

Coeff: -0.916D-02 0.207D+00 0.153D+00 0.649D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=3.06D-06 MaxDP=1.50D-04 DE=-3.35D-05 OVMax= 2.24D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.25D-06 CP: 1.00D+00 1.07D+00 6.47D-01 1.29D+00

E= -1276.01733319155 Delta-E= -0.000001125085 Rises=F Damp=F

DIIS: error= 5.17D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1276.01733319155 IErMin= 5 ErrMin= 5.17D-05

ErrMax= 5.17D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.89D-07 BMatP= 1.79D-06

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

Coeff-Com: -0.440D-02 0.598D-01 0.364D-01 0.411D+00 0.497D+00

Coeff: -0.440D-02 0.598D-01 0.364D-01 0.411D+00 0.497D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=2.00D-06 MaxDP=8.78D-05 DE=-1.13D-06 OVMax= 1.44D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 7.31D-07 CP: 1.00D+00 1.09D+00 6.86D-01 1.62D+00 1.15D+00

E= -1276.01733392896 Delta-E= -0.000000737411 Rises=F Damp=F

DIIS: error= 4.69D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1276.01733392896 IErMin= 6 ErrMin= 4.69D-05

ErrMax= 4.69D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.44D-07 BMatP= 9.89D-07

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

Coeff-Com: 0.210D-02-0.529D-01-0.532D-01-0.630D-01 0.329D-01 0.113D+01

Coeff: 0.210D-02-0.529D-01-0.532D-01-0.630D-01 0.329D-01 0.113D+01

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=3.77D-06 MaxDP=1.95D-04 DE=-7.37D-07 OVMax= 2.98D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.86D-07 CP: 1.00D+00 1.11D+00 7.79D-01 2.17D+00 1.91D+00

CP: 1.66D+00

E= -1276.01733485992 Delta-E= -0.000000930959 Rises=F Damp=F

DIIS: error= 3.05D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1276.01733485992 IErMin= 7 ErrMin= 3.05D-05

ErrMax= 3.05D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.53D-07 BMatP= 2.44D-07

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

Coeff-Com: 0.516D-02-0.873D-01-0.781D-01-0.377D+00-0.510D+00 0.102D+01

Coeff-Com: 0.103D+01

Coeff: 0.516D-02-0.873D-01-0.781D-01-0.377D+00-0.510D+00 0.102D+01

Coeff: 0.103D+01

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=5.21D-06 MaxDP=2.55D-04 DE=-9.31D-07 OVMax= 4.05D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 5.04D-07 CP: 1.00D+00 1.14D+00 9.03D-01 2.97D+00 2.80D+00

CP: 3.00D+00 1.85D+00

E= -1276.01733570865 Delta-E= -0.000000848730 Rises=F Damp=F

DIIS: error= 1.37D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1276.01733570865 IErMin= 8 ErrMin= 1.37D-05

ErrMax= 1.37D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.33D-08 BMatP= 2.44D-07

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

Coeff-Com: 0.157D-02-0.962D-02-0.113D-01-0.154D+00-0.349D+00 0.114D-01

Coeff-Com: 0.554D+00 0.956D+00

Coeff: 0.157D-02-0.962D-02-0.113D-01-0.154D+00-0.349D+00 0.114D-01

Coeff: 0.554D+00 0.956D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=3.33D-06 MaxDP=1.71D-04 DE=-8.49D-07 OVMax= 2.60D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.65D-06 CP: 1.00D+00 1.16D+00 9.82D-01 3.00D+00 3.00D+00

CP: 3.00D+00 2.64D+00 1.24D+00

E= -1276.01733593271 Delta-E= -0.000000224054 Rises=F Damp=F

DIIS: error= 6.93D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1276.01733593271 IErMin= 9 ErrMin= 6.93D-06

ErrMax= 6.93D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.98D-08 BMatP= 6.33D-08

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

Coeff-Com: -0.699D-03 0.242D-01 0.192D-01 0.252D-01-0.578D-01-0.326D+00

Coeff-Com: 0.106D-01 0.619D+00 0.686D+00

Coeff: -0.699D-03 0.242D-01 0.192D-01 0.252D-01-0.578D-01-0.326D+00

Coeff: 0.106D-01 0.619D+00 0.686D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=1.19D-06 MaxDP=5.84D-05 DE=-2.24D-07 OVMax= 9.00D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 2.03D-07 CP: 1.00D+00 1.17D+00 1.01D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.98D+00 1.62D+00 1.39D+00

E= -1276.01733595819 Delta-E= -0.000000025483 Rises=F Damp=F

DIIS: error= 1.83D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1276.01733595819 IErMin=10 ErrMin= 1.83D-06

ErrMax= 1.83D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.95D-09 BMatP= 2.98D-08

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

Coeff-Com: -0.590D-03 0.108D-01 0.956D-02 0.437D-01 0.654D-01-0.115D+00

Coeff-Com: -0.961D-01-0.346D-02 0.254D+00 0.832D+00

Coeff: -0.590D-03 0.108D-01 0.956D-02 0.437D-01 0.654D-01-0.115D+00

Coeff: -0.961D-01-0.346D-02 0.254D+00 0.832D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=1.38D-07 MaxDP=7.30D-06 DE=-2.55D-08 OVMax= 7.25D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.03D-07 CP: 1.00D+00 1.17D+00 1.01D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.66D+00 1.36D+00 9.62D-01

E= -1276.01733596105 Delta-E= -0.000000002857 Rises=F Damp=F

DIIS: error= 1.21D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1276.01733596105 IErMin=11 ErrMin= 1.21D-06

ErrMax= 1.21D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.16D-09 BMatP= 3.95D-09

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

Coeff-Com: -0.101D-03-0.145D-02-0.580D-03 0.131D-01 0.456D-01 0.250D-01

Coeff-Com: -0.364D-01-0.155D+00-0.490D-01 0.390D+00 0.768D+00

Coeff: -0.101D-03-0.145D-02-0.580D-03 0.131D-01 0.456D-01 0.250D-01

Coeff: -0.364D-01-0.155D+00-0.490D-01 0.390D+00 0.768D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=1.00D-07 MaxDP=5.08D-06 DE=-2.86D-09 OVMax= 6.57D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 4.90D-08 CP: 1.00D+00 1.17D+00 1.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.68D+00 1.33D+00 9.88D-01

CP: 1.37D+00

E= -1276.01733596188 Delta-E= -0.000000000834 Rises=F Damp=F

DIIS: error= 7.88D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1276.01733596188 IErMin=12 ErrMin= 7.88D-07

ErrMax= 7.88D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.25D-10 BMatP= 1.16D-09

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

Coeff-Com: 0.110D-03-0.401D-02-0.316D-02-0.361D-02 0.103D-01 0.505D-01

Coeff-Com: 0.268D-02-0.993D-01-0.112D+00-0.681D-02 0.457D+00 0.709D+00

Coeff: 0.110D-03-0.401D-02-0.316D-02-0.361D-02 0.103D-01 0.505D-01

Coeff: 0.268D-02-0.993D-01-0.112D+00-0.681D-02 0.457D+00 0.709D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=4.21D-08 MaxDP=2.77D-06 DE=-8.34D-10 OVMax= 1.51D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 2.13D-08 CP: 1.00D+00 1.17D+00 1.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.69D+00 1.33D+00 1.00D+00

CP: 1.68D+00 1.11D+00

E= -1276.01733596214 Delta-E= -0.000000000264 Rises=F Damp=F

DIIS: error= 3.49D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1276.01733596214 IErMin=13 ErrMin= 3.49D-07

ErrMax= 3.49D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.36D-10 BMatP= 4.25D-10

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

Coeff-Com: 0.903D-04-0.194D-02-0.175D-02-0.593D-02-0.791D-02 0.215D-01

Coeff-Com: 0.873D-02-0.981D-02-0.503D-01-0.991D-01 0.584D-01 0.414D+00

Coeff-Com: 0.674D+00

Coeff: 0.903D-04-0.194D-02-0.175D-02-0.593D-02-0.791D-02 0.215D-01

Coeff: 0.873D-02-0.981D-02-0.503D-01-0.991D-01 0.584D-01 0.414D+00

Coeff: 0.674D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=4.51D-08 MaxDP=2.16D-06 DE=-2.64D-10 OVMax= 3.23D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 1.19D-08 CP: 1.00D+00 1.17D+00 1.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.69D+00 1.34D+00 1.03D+00

CP: 1.76D+00 1.25D+00 9.44D-01

E= -1276.01733596225 Delta-E= -0.000000000103 Rises=F Damp=F

DIIS: error= 1.62D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1276.01733596225 IErMin=14 ErrMin= 1.62D-07

ErrMax= 1.62D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.40D-11 BMatP= 1.36D-10

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

Coeff-Com: 0.130D-04 0.182D-03-0.330D-04-0.130D-02-0.593D-02-0.149D-02

Coeff-Com: -0.284D-04 0.212D-01 0.104D-02-0.438D-01-0.944D-01 0.268D-02

Coeff-Com: 0.298D+00 0.824D+00

Coeff: 0.130D-04 0.182D-03-0.330D-04-0.130D-02-0.593D-02-0.149D-02

Coeff: -0.284D-04 0.212D-01 0.104D-02-0.438D-01-0.944D-01 0.268D-02

Coeff: 0.298D+00 0.824D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=2.28D-08 MaxDP=1.21D-06 DE=-1.03D-10 OVMax= 1.61D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 5.21D-09 CP: 1.00D+00 1.17D+00 1.01D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.70D+00 1.35D+00 1.05D+00

CP: 1.80D+00 1.30D+00 1.13D+00 1.40D+00

E= -1276.01733596229 Delta-E= -0.000000000045 Rises=F Damp=F

DIIS: error= 6.86D-08 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1276.01733596229 IErMin=15 ErrMin= 6.86D-08

ErrMax= 6.86D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.66D-12 BMatP= 2.40D-11

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

Coeff-Com: -0.131D-04 0.530D-03 0.364D-03 0.491D-03-0.173D-02-0.579D-02

Coeff-Com: -0.271D-02 0.145D-01 0.116D-01 0.113D-02-0.596D-01-0.948D-01

Coeff-Com: -0.320D-02 0.424D+00 0.716D+00

Coeff: -0.131D-04 0.530D-03 0.364D-03 0.491D-03-0.173D-02-0.579D-02

Coeff: -0.271D-02 0.145D-01 0.116D-01 0.113D-02-0.596D-01-0.948D-01

Coeff: -0.320D-02 0.424D+00 0.716D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=1.95D-08 MaxDP=9.09D-07 DE=-4.55D-11 OVMax= 1.50D-05

Cycle 16 Pass 1 IDiag 1:

RMSU= 2.46D-09 CP: 1.00D+00 1.17D+00 1.01D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.70D+00 1.36D+00 1.06D+00

CP: 1.81D+00 1.31D+00 1.18D+00 1.64D+00 1.12D+00

E= -1276.01733596230 Delta-E= -0.000000000010 Rises=F Damp=F

DIIS: error= 2.97D-08 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1276.01733596230 IErMin=16 ErrMin= 2.97D-08

ErrMax= 2.97D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.65D-13 BMatP= 6.66D-12

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

Coeff-Com: -0.652D-05 0.176D-03 0.139D-03 0.355D-03 0.278D-04-0.180D-02

Coeff-Com: -0.118D-02 0.292D-02 0.406D-02 0.531D-02-0.965D-02-0.384D-01

Coeff-Com: -0.396D-01 0.584D-01 0.287D+00 0.732D+00

Coeff: -0.652D-05 0.176D-03 0.139D-03 0.355D-03 0.278D-04-0.180D-02

Coeff: -0.118D-02 0.292D-02 0.406D-02 0.531D-02-0.965D-02-0.384D-01

Coeff: -0.396D-01 0.584D-01 0.287D+00 0.732D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=2.58D-09 MaxDP=1.43D-07 DE=-9.55D-12 OVMax= 1.78D-06

Error on total polarization charges = 0.06976

SCF Done: E(UB3LYP) = -1276.01733596 A.U. after 16 cycles

NFock= 16 Conv=0.26D-08 -V/T= 1.9659

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7656 S= 0.5078

<L.S>= 0.000000000000E+00

KE= 1.321017798823D+03 PE=-8.601722383152D+03 EE= 3.243650697002D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.67

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7656, after 0.7501

Leave Link 502 at Tue Sep 17 14:01:49 2019, MaxMem= 2415919104 cpu: 1525.2

(Enter /home/blab/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15325 LenP2D= 41250.

LDataN: DoStor=T MaxTD1= 6 Len= 172

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

GePol: Maximum number of non-zero 1st derivatives = 243

Leave Link 701 at Tue Sep 17 14:01:53 2019, MaxMem= 2415919104 cpu: 71.5

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 14:01:53 2019, MaxMem= 2415919104 cpu: 0.3

(Enter /home/blab/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

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

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

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

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

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Tue Sep 17 14:02:04 2019, MaxMem= 2415919104 cpu: 202.3

(Enter /home/blab/g09/l716.exe)

Dipole = 2.32702746D-13 2.17603713D-13-1.55431223D-15

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.002912901 0.001756373 0.000000000

2 7 -0.004080604 -0.001749200 0.000000000

3 6 0.004048715 -0.001403192 0.000000000

4 6 -0.001235696 0.000867740 -0.000000000

5 6 -0.000092340 -0.001312768 0.000000000

6 7 -0.003168517 0.000702261 0.000000000

7 6 0.001750037 -0.001879587 0.000000000

8 7 0.004692382 0.003146690 0.000000000

9 6 -0.002970015 -0.004482312 -0.000000000

10 6 0.000673821 0.000998760 -0.000000000

11 6 -0.001074964 0.000244695 0.000000000

12 7 -0.001805777 -0.002580842 -0.000000000

13 6 -0.000673821 -0.000998760 0.000000000

14 6 0.001074964 -0.000244695 -0.000000000

15 6 -0.001750037 0.001879587 -0.000000000

16 7 -0.004692382 -0.003146690 0.000000000

17 6 0.002970015 0.004482312 -0.000000000

18 7 0.003168517 -0.000702261 0.000000000

19 7 0.004080604 0.001749200 -0.000000000

20 6 -0.004048715 0.001403192 0.000000000

21 6 0.001235696 -0.000867740 -0.000000000

22 6 0.000092340 0.001312768 0.000000000

23 6 -0.002912901 -0.001756373 0.000000000

24 7 0.001805777 0.002580842 0.000000000

25 30 -0.000000000 0.000000000 -0.000000000

26 6 0.000275989 -0.000367136 0.000000000

27 1 -0.000037370 0.000105285 -0.000000000

28 6 -0.000095945 0.000268433 0.000000000

29 1 -0.000064349 -0.000095526 0.000000000

30 6 0.000095945 -0.000268433 0.000000000

31 1 0.000064349 0.000095526 0.000000000

32 6 -0.000275989 0.000367136 0.000000000

33 1 0.000037370 -0.000105285 -0.000000000

34 1 0.000031011 0.000078340 0.000000000

35 1 -0.000020489 0.000030123 -0.000132953

36 1 -0.000020489 0.000030123 0.000132953

37 1 -0.000012206 -0.000101197 -0.000132096

38 1 -0.000012206 -0.000101197 0.000132096

39 1 0.000049075 0.000035073 0.000000000

40 1 0.000012206 0.000101197 -0.000132096

41 1 0.000012206 0.000101197 0.000132096

42 1 -0.000049075 -0.000035073 0.000000000

43 1 0.000020489 -0.000030123 -0.000132953

44 1 0.000020489 -0.000030123 0.000132953

45 1 -0.000031011 -0.000078340 -0.000000000

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

Cartesian Forces: Max 0.004692382 RMS 0.001463760

Leave Link 716 at Tue Sep 17 14:02:04 2019, MaxMem= 2415919104 cpu: 0.3

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

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

Internal Forces: Max 0.002636283 RMS 0.000550555

Search for a local minimum.

Step number 7 out of a maximum of 270

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

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4 5

6 7

DE= -1.36D-03 DEPred=-3.51D-04 R= 3.88D+00

TightC=F SS= 1.41D+00 RLast= 4.47D-02 DXNew= 5.8050D-01 1.3400D-01

Trust test= 3.88D+00 RLast= 4.47D-02 DXMaxT set to 3.45D-01

ITU= 1 1 1 0 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01328

Eigenvalues --- 0.01330 0.01340 0.01341 0.01608 0.01628

Eigenvalues --- 0.01636 0.01646 0.01770 0.01790 0.01803

Eigenvalues --- 0.01817 0.01886 0.01905 0.01936 0.01948

Eigenvalues --- 0.01996 0.01999 0.02044 0.02048 0.02070

Eigenvalues --- 0.02086 0.02102 0.02109 0.02113 0.02204

Eigenvalues --- 0.02312 0.02317 0.02351 0.02373 0.07149

Eigenvalues --- 0.07181 0.07181 0.07187 0.07187 0.07198

Eigenvalues --- 0.07317 0.07320 0.10610 0.14491 0.14505

Eigenvalues --- 0.15236 0.15907 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 0.16025

Eigenvalues --- 0.16309 0.16462 0.18215 0.19410 0.22065

Eigenvalues --- 0.22092 0.23846 0.23859 0.23901 0.24237

Eigenvalues --- 0.24803 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25001 0.25051 0.25079

Eigenvalues --- 0.27256 0.29380 0.32778 0.33204 0.33210

Eigenvalues --- 0.33247 0.33282 0.33282 0.33481 0.33681

Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33730 0.33927 0.34431 0.34437

Eigenvalues --- 0.34437 0.34444 0.35538 0.35546 0.35549

Eigenvalues --- 0.35682 0.35682 0.35688 0.36569 0.38115

Eigenvalues --- 0.38645 0.41592 0.41776 0.41996 0.44810

Eigenvalues --- 0.48236 0.48951 0.48985 0.51044 0.51359

Eigenvalues --- 0.51365 0.52473 0.53636 0.54002 0.54040

Eigenvalues --- 0.56317 0.56343 0.56567 0.57218

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 1.48510 -0.59922 0.68149 -0.56737

Cosine: 0.963 > 0.710

Length: 0.923

GDIIS step was calculated using 4 of the last 7 vectors.

Iteration 1 RMS(Cart)= 0.00313763 RMS(Int)= 0.00000935

Iteration 2 RMS(Cart)= 0.00001689 RMS(Int)= 0.00000706

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000706

ITry= 1 IFail=0 DXMaxC= 1.53D-02 DCOld= 1.00D+10 DXMaxT= 3.45D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.50D-10 for atom 33.

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

(Linear) (Quad) (Total)

R1 2.59304 -0.00161 -0.00495 -0.00240 -0.00735 2.58568

R2 2.70758 0.00078 0.00344 0.00029 0.00374 2.71132

R3 2.57874 0.00069 -0.00185 0.00490 0.00307 2.58180

R4 2.57553 0.00103 0.00447 0.00025 0.00470 2.58024

R5 3.79812 0.00163 0.00360 0.00384 0.00741 3.80553

R6 2.72732 0.00037 0.00165 -0.00011 0.00154 2.72887

R7 2.58749 -0.00182 -0.00695 0.00116 -0.00578 2.58171

R8 2.62579 -0.00035 -0.00217 0.00132 -0.00084 2.62495

R9 2.82370 0.00026 0.00028 0.00105 0.00133 2.82504

R10 2.04578 -0.00001 -0.00027 0.00013 -0.00013 2.04565

R11 2.50208 0.00101 0.00095 -0.00034 0.00062 2.50270

R12 2.58013 0.00127 0.00412 0.00112 0.00523 2.58536

R13 2.78130 -0.00079 -0.00362 0.00094 -0.00267 2.77864

R14 2.59808 -0.00264 -0.00539 -0.00481 -0.01021 2.58787

R15 3.78473 0.00202 0.00493 0.00659 0.01149 3.79622

R16 2.80248 -0.00016 -0.00147 0.00244 0.00097 2.80344

R17 2.48835 0.00242 0.00611 0.00081 0.00694 2.49529

R18 2.56598 0.00064 0.00247 -0.00094 0.00154 2.56752

R19 2.81672 -0.00007 0.00107 -0.00135 -0.00027 2.81645

R20 2.04486 0.00006 -0.00017 0.00043 0.00026 2.04512

R21 2.48835 0.00242 0.00611 0.00081 0.00694 2.49529

R22 2.56598 0.00064 0.00247 -0.00094 0.00154 2.56752

R23 2.80248 -0.00016 -0.00147 0.00244 0.00097 2.80344

R24 2.81672 -0.00007 0.00107 -0.00135 -0.00027 2.81645

R25 2.78130 -0.00079 -0.00362 0.00094 -0.00267 2.77864

R26 2.04486 0.00006 -0.00017 0.00043 0.00026 2.04512

R27 2.58013 0.00127 0.00412 0.00112 0.00523 2.58536

R28 2.50208 0.00101 0.00095 -0.00034 0.00062 2.50270

R29 2.59808 -0.00264 -0.00539 -0.00481 -0.01021 2.58787

R30 3.78473 0.00202 0.00493 0.00659 0.01149 3.79622

R31 2.58749 -0.00182 -0.00695 0.00116 -0.00578 2.58171

R32 2.57553 0.00103 0.00447 0.00025 0.00470 2.58024

R33 2.59304 -0.00161 -0.00495 -0.00240 -0.00735 2.58568

R34 3.79812 0.00163 0.00360 0.00384 0.00741 3.80553

R35 2.72732 0.00037 0.00165 -0.00011 0.00154 2.72887

R36 2.62579 -0.00035 -0.00217 0.00132 -0.00084 2.62495

R37 2.82370 0.00026 0.00028 0.00105 0.00133 2.82504

R38 2.70758 0.00078 0.00344 0.00029 0.00374 2.71132

R39 2.04578 -0.00001 -0.00027 0.00013 -0.00013 2.04565

R40 2.57874 0.00069 -0.00185 0.00490 0.00307 2.58180

R41 2.06479 -0.00006 -0.00050 0.00019 -0.00031 2.06449

R42 2.07069 -0.00014 -0.00069 0.00006 -0.00063 2.07007

R43 2.07069 -0.00014 -0.00069 0.00006 -0.00063 2.07007

R44 2.06959 -0.00018 -0.00061 -0.00014 -0.00076 2.06883

R45 2.06959 -0.00018 -0.00061 -0.00014 -0.00076 2.06883

R46 2.06311 0.00002 -0.00007 0.00015 0.00008 2.06320

R47 2.06959 -0.00018 -0.00061 -0.00014 -0.00076 2.06883

R48 2.06959 -0.00018 -0.00061 -0.00014 -0.00076 2.06883

R49 2.06311 0.00002 -0.00007 0.00015 0.00008 2.06320

R50 2.07069 -0.00014 -0.00069 0.00006 -0.00063 2.07007

R51 2.07069 -0.00014 -0.00069 0.00006 -0.00063 2.07007

R52 2.06479 -0.00006 -0.00050 0.00019 -0.00031 2.06449

A1 1.88884 0.00001 -0.00064 -0.00019 -0.00084 1.88800

A2 2.20188 0.00067 0.00498 0.00038 0.00536 2.20724

A3 2.19246 -0.00068 -0.00435 -0.00019 -0.00452 2.18794

A4 1.90127 0.00066 0.00311 0.00165 0.00477 1.90604

A5 2.18675 0.00019 0.00072 0.00055 0.00127 2.18803

A6 2.19517 -0.00086 -0.00383 -0.00221 -0.00605 2.18912

A7 1.90292 -0.00088 -0.00433 -0.00121 -0.00555 1.89737

A8 2.21443 0.00019 0.00137 -0.00138 -0.00001 2.21442

A9 2.16583 0.00069 0.00296 0.00259 0.00556 2.17140

A10 1.85128 0.00038 0.00244 0.00025 0.00270 1.85398

A11 2.19006 -0.00029 -0.00249 0.00078 -0.00171 2.18835

A12 2.24185 -0.00009 0.00005 -0.00103 -0.00099 2.24086

A13 1.88047 -0.00017 -0.00059 -0.00050 -0.00108 1.87940

A14 2.18633 -0.00005 -0.00135 0.00025 -0.00110 2.18523

A15 2.21638 0.00022 0.00194 0.00025 0.00218 2.21856

A16 2.16529 0.00138 0.00392 0.00559 0.00952 2.17481

A17 2.23216 -0.00029 -0.00015 -0.00166 -0.00181 2.23035

A18 2.16777 0.00087 0.00514 0.00078 0.00593 2.17370

A19 1.88325 -0.00059 -0.00499 0.00087 -0.00412 1.87913

A20 1.91125 0.00046 0.00364 -0.00043 0.00322 1.91447

A21 2.19711 -0.00117 -0.00422 -0.00287 -0.00709 2.19002

A22 2.17483 0.00071 0.00058 0.00331 0.00387 2.17870

A23 1.88381 0.00043 0.00005 0.00097 0.00100 1.88480

A24 2.23658 0.00002 0.00347 -0.00192 0.00155 2.23813

A25 2.16280 -0.00045 -0.00352 0.00096 -0.00255 2.16025

A26 1.86086 -0.00034 -0.00212 -0.00001 -0.00213 1.85873

A27 2.16585 0.00012 -0.00169 0.00149 -0.00020 2.16565

A28 2.25647 0.00022 0.00381 -0.00149 0.00233 2.25880

A29 1.88561 0.00004 0.00342 -0.00140 0.00203 1.88764

A30 2.17143 -0.00014 -0.00352 0.00085 -0.00268 2.16875

A31 2.22614 0.00011 0.00011 0.00054 0.00064 2.22679

A32 2.18695 -0.00085 -0.00684 0.00021 -0.00662 2.18032

A33 1.86086 -0.00034 -0.00212 -0.00001 -0.00213 1.85873

A34 2.25647 0.00022 0.00381 -0.00149 0.00233 2.25880

A35 2.16585 0.00012 -0.00169 0.00149 -0.00020 2.16565

A36 1.88561 0.00004 0.00342 -0.00140 0.00203 1.88764

A37 2.22614 0.00011 0.00011 0.00054 0.00064 2.22679

A38 2.17143 -0.00014 -0.00352 0.00085 -0.00268 2.16875

A39 1.88325 -0.00059 -0.00499 0.00087 -0.00412 1.87913

A40 2.16777 0.00087 0.00514 0.00078 0.00593 2.17370

A41 2.23216 -0.00029 -0.00015 -0.00166 -0.00181 2.23035

A42 1.91125 0.00046 0.00364 -0.00043 0.00322 1.91447

A43 2.19711 -0.00117 -0.00422 -0.00287 -0.00709 2.19002

A44 2.17483 0.00071 0.00058 0.00331 0.00387 2.17870

A45 2.16280 -0.00045 -0.00352 0.00096 -0.00255 2.16025

A46 2.23658 0.00002 0.00347 -0.00192 0.00155 2.23813

A47 1.88381 0.00043 0.00005 0.00097 0.00100 1.88480

A48 2.16529 0.00138 0.00392 0.00559 0.00952 2.17481

A49 1.90127 0.00066 0.00311 0.00165 0.00477 1.90604

A50 2.19517 -0.00086 -0.00383 -0.00221 -0.00605 2.18912

A51 2.18675 0.00019 0.00072 0.00055 0.00127 2.18803

A52 2.21443 0.00019 0.00137 -0.00138 -0.00001 2.21442

A53 2.16583 0.00069 0.00296 0.00259 0.00556 2.17140

A54 1.90292 -0.00088 -0.00433 -0.00121 -0.00555 1.89737

A55 1.85128 0.00038 0.00244 0.00025 0.00270 1.85398

A56 2.19006 -0.00029 -0.00249 0.00078 -0.00171 2.18835

A57 2.24185 -0.00009 0.00005 -0.00103 -0.00099 2.24086

A58 1.88047 -0.00017 -0.00059 -0.00050 -0.00108 1.87940

A59 2.21638 0.00022 0.00194 0.00025 0.00218 2.21856

A60 2.18633 -0.00005 -0.00135 0.00025 -0.00110 2.18523

A61 1.88884 0.00001 -0.00064 -0.00019 -0.00084 1.88800

A62 2.20188 0.00067 0.00498 0.00038 0.00536 2.20724

A63 2.19246 -0.00068 -0.00435 -0.00019 -0.00452 2.18794

A64 2.18695 -0.00085 -0.00684 0.00021 -0.00662 2.18032

A65 1.56221 0.00074 0.00291 0.00252 0.00544 1.56765

A66 1.57938 -0.00074 -0.00291 -0.00252 -0.00544 1.57395

A67 1.57938 -0.00074 -0.00291 -0.00252 -0.00544 1.57395

A68 1.56221 0.00074 0.00291 0.00252 0.00544 1.56765

A69 1.94191 -0.00009 -0.00103 -0.00005 -0.00108 1.94082

A70 1.94991 0.00002 -0.00037 0.00036 -0.00001 1.94990

A71 1.94991 0.00002 -0.00037 0.00036 -0.00001 1.94990

A72 1.88030 0.00004 0.00083 -0.00031 0.00051 1.88081

A73 1.88030 0.00004 0.00083 -0.00031 0.00051 1.88081

A74 1.85735 -0.00004 0.00027 -0.00010 0.00018 1.85753

A75 1.93992 0.00002 0.00036 -0.00051 -0.00015 1.93977

A76 1.93992 0.00002 0.00036 -0.00051 -0.00015 1.93977

A77 1.94452 0.00004 0.00013 0.00016 0.00028 1.94480

A78 1.85751 0.00000 -0.00012 0.00072 0.00059 1.85811

A79 1.88938 -0.00004 -0.00038 0.00010 -0.00028 1.88910

A80 1.88938 -0.00004 -0.00038 0.00010 -0.00028 1.88910

A81 1.93992 0.00002 0.00036 -0.00051 -0.00015 1.93977

A82 1.93992 0.00002 0.00036 -0.00051 -0.00015 1.93977

A83 1.94452 0.00004 0.00013 0.00016 0.00028 1.94480

A84 1.85751 0.00000 -0.00012 0.00072 0.00059 1.85811

A85 1.88938 -0.00004 -0.00038 0.00010 -0.00028 1.88910

A86 1.88938 -0.00004 -0.00038 0.00010 -0.00028 1.88910

A87 1.94991 0.00002 -0.00037 0.00036 -0.00001 1.94990

A88 1.94991 0.00002 -0.00037 0.00036 -0.00001 1.94990

A89 1.94191 -0.00009 -0.00103 -0.00005 -0.00108 1.94082

A90 1.85735 -0.00004 0.00027 -0.00010 0.00018 1.85753

A91 1.88030 0.00004 0.00083 -0.00031 0.00051 1.88081

A92 1.88030 0.00004 0.00083 -0.00031 0.00051 1.88081

A93 3.14159 -0.00000 -0.00000 -0.00000 -0.00000 3.14159

A94 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

A95 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

A96 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D2 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D3 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D4 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D5 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

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D7 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

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D10 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D11 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D25 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D27 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D28 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D29 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D30 1.03928 -0.00001 -0.00007 0.00018 0.00010 1.03938

D31 -1.03928 0.00001 0.00007 -0.00018 -0.00010 -1.03938

D32 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D33 -2.10232 -0.00001 -0.00007 0.00018 0.00010 -2.10221

D34 2.10232 0.00001 0.00007 -0.00018 -0.00010 2.10221

D35 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D36 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D37 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D38 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D39 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

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D42 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D43 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D44 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D45 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D46 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

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D48 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D49 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

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D53 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

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D57 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D58 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D59 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D60 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D61 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D62 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D63 1.03276 0.00001 0.00016 0.00012 0.00027 1.03303

D64 -1.03276 -0.00001 -0.00016 -0.00012 -0.00027 -1.03303

D65 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D66 -2.10883 0.00001 0.00016 0.00012 0.00027 -2.10856

D67 2.10883 -0.00001 -0.00016 -0.00012 -0.00027 2.10856

D68 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D69 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D70 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D71 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D72 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D73 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D74 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D75 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D76 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D77 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D78 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D79 -2.10883 0.00001 0.00016 0.00012 0.00027 -2.10856

D80 2.10883 -0.00001 -0.00016 -0.00012 -0.00027 2.10856

D81 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D82 1.03276 0.00001 0.00016 0.00012 0.00027 1.03303

D83 -1.03276 -0.00001 -0.00016 -0.00012 -0.00027 -1.03303

D84 3.14159 0.00000 -0.00000 -0.00000 0.00000 3.14159

D85 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D86 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D87 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D88 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

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D90 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D91 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D92 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

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D94 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D95 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D96 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D97 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D98 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D99 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D100 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D101 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D102 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D103 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D104 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D105 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D106 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D107 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D108 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D109 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D110 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D111 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D112 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D113 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D114 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D115 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D116 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D117 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D118 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D119 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D120 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D121 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D122 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D123 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

D124 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D125 1.03928 -0.00001 -0.00007 0.00018 0.00010 1.03938

D126 -1.03928 0.00001 0.00007 -0.00018 -0.00010 -1.03938

D127 3.14159 0.00000 -0.00000 -0.00000 0.00000 3.14159

D128 -2.10232 -0.00001 -0.00007 0.00018 0.00010 -2.10221

D129 2.10232 0.00001 0.00007 -0.00018 -0.00010 2.10221

D130 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D131 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D132 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D133 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D134 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D135 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D136 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

Item Value Threshold Converged?

Maximum Force 0.002636 0.000450 NO

RMS Force 0.000551 0.000300 NO

Maximum Displacement 0.015350 0.001800 NO

RMS Displacement 0.003133 0.001200 NO

Predicted change in Energy=-2.087123D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:02:05 2019, MaxMem= 2415919104 cpu: 1.8

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.073189 -2.195240 -0.000000

2 7 0 -0.743775 -1.871414 -0.000000

3 6 0 -0.002168 -3.017861 -0.000000

4 6 0 -0.898965 -4.149694 -0.000000

5 6 0 -2.185371 -3.625615 -0.000000

6 7 0 1.360723 -3.112669 -0.000000

7 6 0 2.186733 -2.077454 -0.000000

8 7 0 1.864487 -0.747834 -0.000000

9 6 0 3.008890 0.004308 -0.000000

10 6 0 4.166763 -0.923140 -0.000000

11 6 0 3.653466 -2.181123 -0.000000

12 7 0 -3.122162 -1.319889 -0.000000

13 6 0 -4.166763 0.923140 -0.000000

14 6 0 -3.653466 2.181123 -0.000000

15 6 0 -2.186733 2.077454 -0.000000

16 7 0 -1.864487 0.747834 -0.000000

17 6 0 -3.008890 -0.004308 -0.000000

18 7 0 -1.360723 3.112669 -0.000000

19 7 0 0.743775 1.871414 -0.000000

20 6 0 0.002168 3.017861 -0.000000

21 6 0 0.898965 4.149694 -0.000000

22 6 0 2.185371 3.625615 -0.000000

23 6 0 2.073189 2.195240 -0.000000

24 7 0 3.122162 1.319889 -0.000000

25 30 0 0.000000 -0.000000 -0.000000

26 6 0 -0.481242 -5.585092 -0.000000

27 1 0 -3.115978 -4.178608 -0.000000

28 6 0 5.590336 -0.481850 -0.000000

29 1 0 4.198135 -3.116300 -0.000000

30 6 0 -5.590336 0.481850 -0.000000

31 1 0 -4.198135 3.116300 -0.000000

32 6 0 0.481242 5.585092 -0.000000

33 1 0 3.115978 4.178608 -0.000000

34 1 0 -1.348813 -6.249043 -0.000000

35 1 0 0.127197 -5.830246 0.877309

36 1 0 0.127197 -5.830246 -0.877309

37 1 0 5.812609 0.134630 0.876976

38 1 0 5.812609 0.134630 -0.876976

39 1 0 6.272254 -1.334498 -0.000000

40 1 0 -5.812609 -0.134630 0.876976

41 1 0 -5.812609 -0.134630 -0.876976

42 1 0 -6.272254 1.334498 -0.000000

43 1 0 -0.127197 5.830246 0.877309

44 1 0 -0.127197 5.830246 -0.877309

45 1 0 1.348813 6.249043 -0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.368285 0.000000

3 C 2.228415 1.365402 0.000000

4 C 2.280064 2.283560 1.444053 0.000000

5 C 1.434767 2.270555 2.266217 1.389065 0.000000

6 N 3.554353 2.443282 1.366185 2.486284 3.583001

7 C 4.261550 2.937743 2.382363 3.716949 4.638114

8 N 4.195268 2.839976 2.938950 4.382844 4.968197

9 C 5.537647 4.195334 4.266143 5.703250 6.336931

10 C 6.368299 5.001260 4.665602 6.006018 6.903114

11 C 5.726673 4.408135 3.750173 4.959829 6.014863

12 N 1.366230 2.441496 3.552108 3.598667 2.488764

13 C 3.755974 4.418866 5.733702 6.034248 4.961560

14 C 4.652938 4.988924 6.353064 6.904095 5.989450

15 C 4.274202 4.204246 5.543876 6.358909 5.703069

16 N 2.950464 2.848939 4.201034 4.991794 4.385204

17 C 2.382377 2.935444 4.256980 4.651453 3.713765

18 N 5.355512 5.022122 6.279257 7.277028 6.788558

19 N 4.947015 4.027600 4.945851 6.241180 6.228742

20 C 5.611018 4.945851 6.035724 7.223980 6.994362

21 C 7.006560 6.241180 7.223980 8.491901 8.364721

22 C 7.212328 6.228742 6.994362 8.364721 8.466624

23 C 6.038937 4.947015 5.611018 7.006560 7.212328

24 N 6.272783 5.012972 5.345794 6.788652 7.254510

25 Zn 3.019468 2.013800 3.017862 4.245951 4.233312

26 C 3.745049 3.722946 2.611549 1.494945 2.596845

27 H 2.240795 3.309153 3.323123 2.217202 1.082511

28 C 7.852727 6.484740 6.140640 7.454133 8.387185

29 H 6.338601 5.096295 4.201457 5.200801 6.403793

30 C 4.420083 5.387671 6.593602 6.592432 5.335265

31 H 5.720826 6.067116 7.431963 7.979925 7.035953

32 C 8.188936 7.556464 8.616524 9.832142 9.588949

33 H 8.219087 7.176382 7.842959 9.245560 9.434522

34 H 4.118014 4.419243 3.500570 2.147005 2.753581

35 H 4.338737 4.147363 2.948884 2.155675 3.313313

36 H 4.338737 4.147363 2.948884 2.155675 3.313313

37 H 8.269413 6.912270 6.672250 8.010602 8.881228

38 H 8.269413 6.912270 6.672250 8.010602 8.881228

39 H 8.389714 7.036544 6.496314 7.704007 8.762457

40 H 4.358723 5.429418 6.545481 6.405757 5.110079

41 H 4.358723 5.429418 6.545481 6.405757 5.110079

42 H 5.485544 6.390771 7.632628 7.677799 6.426922

43 H 8.304516 7.775951 8.892374 10.048110 9.716947

44 H 8.304516 7.775951 8.892374 10.048110 9.716947

45 H 9.111312 8.385747 9.364863 10.638902 10.488056

6 7 8 9 10

6 N 0.000000

7 C 1.324373 0.000000

8 N 2.417897 1.368113 0.000000

9 C 3.525904 2.238230 1.369444 0.000000

10 C 3.559199 2.291933 2.308941 1.483519 0.000000

11 C 2.474763 1.470392 2.292328 2.278506 1.358674

12 N 4.828076 5.362674 5.019354 6.272424 7.299715

13 C 6.844038 7.026413 6.258445 7.234242 8.535596

14 C 7.291525 7.227961 6.247127 7.008960 8.413824

15 C 6.286639 6.032452 4.939093 5.593965 7.026413

16 N 5.030453 4.939093 4.017744 4.929771 6.258445

17 C 5.362409 5.593965 4.929771 6.017787 7.234242

18 N 6.794196 6.286639 5.030453 5.362409 6.844038

19 N 5.022122 4.204246 2.848939 2.935444 4.418866

20 C 6.279257 5.543876 4.201034 4.256980 5.733702

21 C 7.277028 6.358909 4.991794 4.651453 6.034248

22 C 6.788558 5.703069 4.385204 3.713765 4.961560

23 C 5.355512 4.274202 2.950464 2.382377 3.755974

24 N 4.769721 3.523772 2.420170 1.320449 2.474342

25 Zn 3.397098 3.016226 2.008872 3.008893 4.267798

26 C 3.083133 4.406996 5.376013 6.589569 6.583141

27 H 4.601856 5.703823 6.047747 7.416927 7.977242

28 C 4.981048 3.759051 3.735331 2.626825 1.490402

29 H 2.837415 2.263833 3.324989 3.339536 2.193385

30 C 7.825457 8.187359 7.555561 8.612476 9.857737

31 H 8.348710 8.230531 7.189362 7.850205 9.289166

32 C 8.742112 7.850052 6.482230 6.126513 7.479314

33 H 7.499577 6.324699 5.082918 4.175674 5.208837

34 H 4.144686 5.468294 6.370919 7.621940 7.667256

35 H 3.110705 4.369761 5.442313 6.566266 6.416187

36 H 3.110705 4.369761 5.442313 6.566266 6.416187

37 H 5.579725 4.336978 4.139504 2.940563 2.144009

38 H 5.579725 4.336978 4.139504 2.940563 2.144009

39 H 5.223508 4.152525 4.446638 3.527314 2.145299

40 H 7.816296 8.278474 7.751316 8.866072 10.048816

41 H 7.816296 8.278474 7.751316 8.866072 10.048816

42 H 8.834004 9.121178 8.398968 9.375983 10.680356

43 H 9.108200 8.285872 6.928753 6.674300 8.050838

44 H 9.108200 8.285872 6.928753 6.674300 8.050838

45 H 9.361720 8.368553 7.015854 6.461624 7.705910

11 12 13 14 15

11 C 0.000000

12 N 6.830144 0.000000

13 C 8.413824 2.474342 0.000000

14 C 8.510021 3.541098 1.358674 0.000000

15 C 7.227961 3.523772 2.291933 1.470392 0.000000

16 N 6.247127 2.420170 2.308941 2.292328 1.368113

17 C 7.008960 1.320449 1.483519 2.278506 2.238230

18 N 7.291525 4.769721 3.559199 2.474763 1.324373

19 N 4.988924 5.012972 5.001260 4.408135 2.937743

20 C 6.353064 5.345794 4.665602 3.750173 2.382363

21 C 6.904095 6.788652 6.006018 4.959829 3.716949

22 C 5.989450 7.254510 6.903114 6.014863 4.638114

23 C 4.652938 6.272783 6.368299 5.726673 4.261550

24 N 3.541098 6.779382 7.299715 6.830144 5.362674

25 Zn 4.255011 3.389691 4.267798 4.255011 3.016226

26 C 5.355634 5.016614 7.479314 8.389106 7.850052

27 H 7.057997 2.858726 5.208837 6.382404 6.324699

28 C 2.576624 8.752710 9.857737 9.619735 8.187359

29 H 1.082229 7.537496 9.289166 9.471555 8.230531

30 C 9.619735 3.055838 1.490402 2.576624 3.759051

31 H 9.471555 4.564810 2.193385 1.082229 2.263833

32 C 8.389106 7.788664 6.583141 5.355634 4.406996

33 H 6.382404 8.315520 7.977242 7.057997 5.703823

34 H 6.447540 5.238447 7.705910 8.739516 8.368553

35 H 5.149791 5.627729 8.050838 8.901974 8.285872

36 H 5.149791 5.627729 8.050838 8.901974 8.285872

37 H 3.285377 9.094770 10.048816 9.724392 8.278474

38 H 3.285377 9.094770 10.048816 9.724392 8.278474

39 H 2.752240 9.394428 10.680356 10.529935 9.121178

40 H 9.724392 3.067968 2.144009 3.285377 4.336978

41 H 9.724392 3.067968 2.144009 3.285377 4.336978

42 H 10.529935 4.119326 2.145299 2.752240 4.152525

43 H 8.901974 7.801534 6.416187 5.149791 4.369761

44 H 8.901974 7.801534 6.416187 5.149791 4.369761

45 H 8.739516 8.790811 7.667256 6.447540 5.468294

16 17 18 19 20

16 N 0.000000

17 C 1.369444 0.000000

18 N 2.417897 3.525904 0.000000

19 N 2.839976 4.195334 2.443282 0.000000

20 C 2.938950 4.266143 1.366185 1.365402 0.000000

21 C 4.382844 5.703250 2.486284 2.283560 1.444053

22 C 4.968197 6.336931 3.583001 2.270555 2.266217

23 C 4.195268 5.537647 3.554353 1.368285 2.228415

24 N 5.019354 6.272424 4.828076 2.441496 3.552108

25 Zn 2.008872 3.008893 3.397098 2.013800 3.017862

26 C 6.482230 6.126513 8.742112 7.556464 8.616524

27 H 5.082918 4.175674 7.499577 7.176382 7.842959

28 C 7.555561 8.612476 7.825457 5.387671 6.593602

29 H 7.189362 7.850205 8.348710 6.067116 7.431963

30 C 3.735331 2.626825 4.981048 6.484740 6.140640

31 H 3.324989 3.339536 2.837415 5.096295 4.201457

32 C 5.376013 6.589569 3.083133 3.722946 2.611549

33 H 6.047747 7.416927 4.601856 3.309153 3.323123

34 H 7.015854 6.461624 9.361720 8.385747 9.364863

35 H 6.928753 6.674300 9.108200 7.775951 8.892374

36 H 6.928753 6.674300 9.108200 7.775951 8.892374

37 H 7.751316 8.866072 7.816296 5.429418 6.545481

38 H 7.751316 8.866072 7.816296 5.429418 6.545481

39 H 8.398968 9.375983 8.834004 6.390771 7.632628

40 H 4.139504 2.940563 5.579725 6.912270 6.672250

41 H 4.139504 2.940563 5.579725 6.912270 6.672250

42 H 4.446638 3.527314 5.223508 7.036544 6.496314

43 H 5.442313 6.566266 3.110705 4.147363 2.948884

44 H 5.442313 6.566266 3.110705 4.147363 2.948884

45 H 6.370919 7.621940 4.144686 4.419243 3.500570

21 22 23 24 25

21 C 0.000000

22 C 1.389065 0.000000

23 C 2.280064 1.434767 0.000000

24 N 3.598667 2.488764 1.366230 0.000000

25 Zn 4.245951 4.233312 3.019468 3.389691 0.000000

26 C 9.832142 9.588949 8.188936 7.788664 5.605787

27 H 9.245560 9.434522 8.219087 8.315520 5.212493

28 C 6.592432 5.335265 4.420083 3.055838 5.611064

29 H 7.979925 7.035953 5.720826 4.564810 5.228352

30 C 7.454133 8.387185 7.852727 8.752710 5.611064

31 H 5.200801 6.403793 6.338601 7.537496 5.228352

32 C 1.494945 2.596845 3.745049 5.016614 5.605787

33 H 2.217202 1.082511 2.240795 2.858726 5.212493

34 H 10.638902 10.488056 9.111312 8.790811 6.392952

35 H 10.048110 9.716947 8.304516 7.801534 5.897256

36 H 10.048110 9.716947 8.304516 7.801534 5.897256

37 H 6.405757 5.110079 4.358723 3.067968 5.879935

38 H 6.405757 5.110079 4.358723 3.067968 5.879935

39 H 7.677799 6.426922 5.485544 4.119326 6.412648

40 H 8.010602 8.881228 8.269413 9.094770 5.879935

41 H 8.010602 8.881228 8.269413 9.094770 5.879935

42 H 7.704007 8.762457 8.389714 9.394428 6.412648

43 H 2.155675 3.313313 4.338737 5.627729 5.897256

44 H 2.155675 3.313313 4.338737 5.627729 5.897256

45 H 2.147005 2.753581 4.118014 5.238447 6.392952

26 27 28 29 30

26 C 0.000000

27 H 2.986642 0.000000

28 C 7.931402 9.458643 0.000000

29 H 5.290700 7.390856 2.979690 0.000000

30 C 7.931621 5.276582 11.222127 10.428847 0.000000

31 H 9.462004 7.374738 10.428847 10.456705 2.979690

32 C 11.211573 10.405279 7.931621 9.462004 7.931402

33 H 10.405279 10.424987 5.276582 7.374738 9.458643

34 H 1.092479 2.722053 9.022877 6.370456 7.955843

35 H 1.095432 3.743763 7.695512 4.970685 8.561683

36 H 1.095432 3.743763 7.695512 4.970685 8.561683

37 H 8.549671 9.954536 1.094779 3.734188 11.441888

38 H 8.549671 9.954536 1.094779 3.734188 11.441888

39 H 7.979804 9.809581 1.091797 2.734372 12.000840

40 H 7.674639 4.939095 11.441888 10.482101 1.094779

41 H 7.674639 4.939095 11.441888 10.482101 1.094779

42 H 9.023111 6.352670 12.000840 11.377111 1.091797

43 H 11.454474 10.482350 8.561683 9.975914 7.695512

44 H 11.454474 10.482350 8.561683 9.975914 7.695512

45 H 11.974801 11.343292 7.955843 9.789193 9.022877

31 32 33 34 35

31 H 0.000000

32 C 5.290700 0.000000

33 H 7.390856 2.986642 0.000000

34 H 9.789193 11.974801 11.343292 0.000000

35 H 9.975914 11.454474 10.482350 1.767390 0.000000

36 H 9.975914 11.454474 10.482350 1.767390 1.754618

37 H 10.482101 7.674639 4.939095 9.633604 8.240368

38 H 10.482101 7.674639 4.939095 9.633604 8.425033

39 H 11.377111 9.023111 6.352670 9.068265 7.664409

40 H 3.734188 8.549671 9.954536 7.621064 8.229298

41 H 3.734188 8.549671 9.954536 7.621064 8.414206

42 H 2.734372 7.979804 9.809581 9.041591 9.646564

43 H 4.970685 1.095432 3.743763 12.172562 11.663268

44 H 4.970685 1.095432 3.743763 12.172562 11.794511

45 H 6.370456 1.092479 2.722053 12.785904 12.172562

36 37 38 39 40

36 H 0.000000

37 H 8.425033 0.000000

38 H 8.240368 1.753953 0.000000

39 H 7.664409 1.771637 1.771637 0.000000

40 H 8.414206 11.628336 11.759870 12.175906 0.000000

41 H 8.229298 11.759870 11.628336 12.175906 1.753953

42 H 9.646564 12.175906 12.175906 12.825296 1.771637

43 H 11.794511 8.229298 8.414206 9.646564 8.240368

44 H 11.663268 8.414206 8.229298 9.646564 8.425033

45 H 12.172562 7.621064 7.621064 9.041591 9.633604

41 42 43 44 45

41 H 0.000000

42 H 1.771637 0.000000

43 H 8.425033 7.664409 0.000000

44 H 8.240368 7.664409 1.754618 0.000000

45 H 9.633604 9.068265 1.767390 1.767390 0.000000

Stoichiometry C20H16N8Zn(1-,2)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=3 Diff= 3.14D-01

Largest Abelian subgroup C2H NOp 4

Largest concise Abelian subgroup C2H NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.947611 0.654813 0.000000

2 7 0 -1.988106 -0.320664 0.000000

3 6 0 -2.592328 -1.545097 0.000000

4 6 0 -4.023849 -1.355262 0.000000

5 6 0 -4.233274 0.017924 0.000000

6 7 0 -1.975113 -2.763911 0.000000

7 6 0 -0.662836 -2.942494 0.000000

8 7 0 0.313628 -1.984239 0.000000

9 6 0 1.546059 -2.581306 0.000000

10 6 0 1.343255 -4.050897 0.000000

11 6 0 0.000000 -4.255011 0.000000

12 7 0 -2.733716 2.004196 0.000000

13 6 0 -1.343255 4.050897 0.000000

14 6 0 0.000000 4.255011 0.000000

15 6 0 0.662836 2.942494 0.000000

16 7 0 -0.313628 1.984239 0.000000

17 6 0 -1.546059 2.581306 0.000000

18 7 0 1.975113 2.763911 0.000000

19 7 0 1.988106 0.320664 0.000000

20 6 0 2.592328 1.545097 0.000000

21 6 0 4.023849 1.355262 0.000000

22 6 0 4.233274 -0.017924 0.000000

23 6 0 2.947611 -0.654813 0.000000

24 7 0 2.733716 -2.004196 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -5.042195 -2.449717 0.000000

27 1 0 -5.185119 0.533503 0.000000

28 6 0 2.451883 -5.047009 0.000000

29 1 0 -0.523770 -5.202051 0.000000

30 6 0 -2.451883 5.047009 0.000000

31 1 0 0.523770 5.202051 0.000000

32 6 0 5.042195 2.449717 0.000000

33 1 0 5.185119 -0.533503 0.000000

34 1 0 -6.056999 -2.045140 0.000000

35 1 0 -4.940805 -3.097806 0.877309

36 1 0 -4.940805 -3.097806 -0.877309

37 1 0 3.095147 -4.921850 0.876976

38 1 0 3.095147 -4.921850 -0.876976

39 1 0 2.069329 -6.069591 0.000000

40 1 0 -3.095147 4.921850 0.876976

41 1 0 -3.095147 4.921850 -0.876976

42 1 0 -2.069329 6.069591 0.000000

43 1 0 4.940805 3.097806 0.877309

44 1 0 4.940805 3.097806 -0.877309

45 1 0 6.056999 2.045140 0.000000

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

Rotational constants (GHZ): 0.1826729 0.1815829 0.0912672

Leave Link 202 at Tue Sep 17 14:02:05 2019, MaxMem= 2415919104 cpu: 0.2

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 229 symmetry adapted cartesian basis functions of AG symmetry.

There are 82 symmetry adapted cartesian basis functions of BG symmetry.

There are 78 symmetry adapted cartesian basis functions of AU symmetry.

There are 218 symmetry adapted cartesian basis functions of BU symmetry.

There are 212 symmetry adapted basis functions of AG symmetry.

There are 82 symmetry adapted basis functions of BG symmetry.

There are 78 symmetry adapted basis functions of AU symmetry.

There are 204 symmetry adapted basis functions of BU symmetry.

576 basis functions, 1015 primitive gaussians, 607 cartesian basis functions

103 alpha electrons 102 beta electrons

nuclear repulsion energy 2759.6602712002 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= 45 NActive= 45 NUniq= 21 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1141395012 Hartrees.

Nuclear repulsion after empirical dispersion term = 2759.5461316990 Hartrees.

No density basis found on file 724.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

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 = 45

GePol: Total number of spheres = 45

GePol: Number of exposed spheres = 45 (100.00%)

GePol: Number of points = 3616

GePol: Average weight of points = 0.10

GePol: Minimum weight of points = 0.12D-09

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 280

GePol: Fraction of low-weight points (<1% of avg) = 7.74%

GePol: Cavity surface area = 378.960 Ang\*\*2

GePol: Cavity volume = 378.293 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0106361467 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2759.5354955522 Hartrees.

Leave Link 301 at Tue Sep 17 14:02:05 2019, MaxMem= 2415919104 cpu: 2.2

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15313 LenP2D= 41232.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.79D-04 NBF= 212 82 78 204

NBsUse= 576 1.00D-06 EigRej= -1.00D+00 NBFU= 212 82 78 204

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= 594 594 594 594 594 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Tue Sep 17 14:02:05 2019, MaxMem= 2415919104 cpu: 12.3

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:02:06 2019, MaxMem= 2415919104 cpu: 1.5

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

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

B after Tr= -0.000000 -0.000000 0.000000

Rot= 0.993826 0.000000 -0.000000 0.110954 Ang= 12.74 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-BG.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7656 S= 0.5078

Leave Link 401 at Tue Sep 17 14:02:07 2019, MaxMem= 2415919104 cpu: 20.8

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1141655 IEndB= 1141655 NGot= 2415919104 MDV= 2415163146

LenX= 2415163146 LenY= 2414794090

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= 670000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 39226368.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.55D-15 for 3606.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.33D-15 for 3358 2090.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.33D-15 for 3595.

Iteration 1 A^-1\*A deviation from orthogonality is 2.23D-12 for 1975 1971.

E= -1276.01555537722

DIIS: error= 6.68D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1276.01555537722 IErMin= 1 ErrMin= 6.68D-04

ErrMax= 6.68D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.47D-04 BMatP= 6.47D-04

IDIUse=3 WtCom= 9.93D-01 WtEn= 6.68D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.294 Goal= None Shift= 0.000

Gap= 0.342 Goal= None Shift= 0.000

RMSDP=3.86D-05 MaxDP=1.51D-03 OVMax= 7.90D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.86D-05 CP: 1.00D+00

E= -1276.01574095069 Delta-E= -0.000185573474 Rises=F Damp=F

DIIS: error= 3.25D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1276.01574095069 IErMin= 2 ErrMin= 3.25D-04

ErrMax= 3.25D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.62D-05 BMatP= 6.47D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.25D-03

Coeff-Com: 0.130D+00 0.870D+00

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

Coeff: 0.129D+00 0.871D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=2.00D-05 MaxDP=9.93D-04 DE=-1.86D-04 OVMax= 1.05D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.99D-05 CP: 1.00D+00 1.01D+00

E= -1276.01572280957 Delta-E= 0.000018141117 Rises=F Damp=F

DIIS: error= 5.57D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1276.01574095069 IErMin= 2 ErrMin= 3.25D-04

ErrMax= 5.57D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.94D-04 BMatP= 7.62D-05

IDIUse=3 WtCom= 2.98D-01 WtEn= 7.02D-01

Coeff-Com: -0.159D-01 0.626D+00 0.389D+00

Coeff-En: 0.000D+00 0.634D+00 0.366D+00

Coeff: -0.473D-02 0.632D+00 0.373D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.11D-05 MaxDP=4.94D-04 DE= 1.81D-05 OVMax= 1.90D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 7.32D-06 CP: 1.00D+00 1.08D+00 6.00D-01

E= -1276.01576463942 Delta-E= -0.000041829846 Rises=F Damp=F

DIIS: error= 1.05D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1276.01576463942 IErMin= 4 ErrMin= 1.05D-04

ErrMax= 1.05D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.89D-06 BMatP= 7.62D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.05D-03

Coeff-Com: -0.105D-01 0.240D+00 0.124D+00 0.646D+00

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

Coeff: -0.105D-01 0.240D+00 0.124D+00 0.647D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=4.12D-06 MaxDP=2.13D-04 DE=-4.18D-05 OVMax= 3.06D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.68D-06 CP: 1.00D+00 1.10D+00 7.23D-01 1.22D+00

E= -1276.01576671343 Delta-E= -0.000002074007 Rises=F Damp=F

DIIS: error= 7.60D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1276.01576671343 IErMin= 5 ErrMin= 7.60D-05

ErrMax= 7.60D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.77D-06 BMatP= 2.89D-06

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

Coeff-Com: -0.209D-02 0.243D-01-0.336D-01 0.367D+00 0.644D+00

Coeff: -0.209D-02 0.243D-01-0.336D-01 0.367D+00 0.644D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=3.88D-06 MaxDP=1.83D-04 DE=-2.07D-06 OVMax= 3.00D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 9.34D-07 CP: 1.00D+00 1.13D+00 8.15D-01 1.62D+00 1.45D+00

E= -1276.01576863147 Delta-E= -0.000001918044 Rises=F Damp=F

DIIS: error= 6.21D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1276.01576863147 IErMin= 6 ErrMin= 6.21D-05

ErrMax= 6.21D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.63D-07 BMatP= 1.77D-06

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

Coeff-Com: 0.420D-02-0.839D-01-0.967D-01-0.237D+00-0.132D+00 0.155D+01

Coeff: 0.420D-02-0.839D-01-0.967D-01-0.237D+00-0.132D+00 0.155D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=7.69D-06 MaxDP=3.79D-04 DE=-1.92D-06 OVMax= 6.03D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 7.55D-07 CP: 1.00D+00 1.18D+00 1.02D+00 2.33D+00 2.64D+00

CP: 2.28D+00

E= -1276.01577127638 Delta-E= -0.000002644913 Rises=F Damp=F

DIIS: error= 3.78D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1276.01577127638 IErMin= 7 ErrMin= 3.78D-05

ErrMax= 3.78D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.00D-07 BMatP= 7.63D-07

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

Coeff-Com: 0.569D-02-0.801D-01-0.710D-01-0.455D+00-0.636D+00 0.125D+01

Coeff-Com: 0.992D+00

Coeff: 0.569D-02-0.801D-01-0.710D-01-0.455D+00-0.636D+00 0.125D+01

Coeff: 0.992D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=8.53D-06 MaxDP=4.25D-04 DE=-2.64D-06 OVMax= 6.67D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.87D-06 CP: 1.00D+00 1.24D+00 1.24D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.61D+00

E= -1276.01577284659 Delta-E= -0.000001570209 Rises=F Damp=F

DIIS: error= 1.09D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1276.01577284659 IErMin= 8 ErrMin= 1.09D-05

ErrMax= 1.09D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.02D-07 BMatP= 4.00D-07

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

Coeff-Com: 0.449D-03 0.104D-01 0.114D-01-0.941D-01-0.261D+00-0.121D+00

Coeff-Com: 0.546D+00 0.908D+00

Coeff: 0.449D-03 0.104D-01 0.114D-01-0.941D-01-0.261D+00-0.121D+00

Coeff: 0.546D+00 0.908D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=3.94D-06 MaxDP=1.97D-04 DE=-1.57D-06 OVMax= 3.05D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.93D-06 CP: 1.00D+00 1.26D+00 1.34D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.19D+00 1.90D+00

E= -1276.01577307439 Delta-E= -0.000000227801 Rises=F Damp=F

DIIS: error= 4.17D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1276.01577307439 IErMin= 9 ErrMin= 4.17D-06

ErrMax= 4.17D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.96D-08 BMatP= 1.02D-07

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

Coeff-Com: -0.856D-03 0.221D-01 0.219D-01 0.377D-01-0.425D-02-0.296D+00

Coeff-Com: 0.613D-01 0.494D+00 0.664D+00

Coeff: -0.856D-03 0.221D-01 0.219D-01 0.377D-01-0.425D-02-0.296D+00

Coeff: 0.613D-01 0.494D+00 0.664D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=6.56D-07 MaxDP=3.26D-05 DE=-2.28D-07 OVMax= 4.68D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 2.08D-07 CP: 1.00D+00 1.26D+00 1.36D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.36D+00 2.04D+00 1.14D+00

E= -1276.01577308779 Delta-E= -0.000000013394 Rises=F Damp=F

DIIS: error= 2.40D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1276.01577308779 IErMin=10 ErrMin= 2.40D-06

ErrMax= 2.40D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.54D-09 BMatP= 2.96D-08

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

Coeff-Com: -0.576D-03 0.812D-02 0.801D-02 0.524D-01 0.932D-01-0.103D+00

Coeff-Com: -0.147D+00-0.211D-02 0.337D+00 0.754D+00

Coeff: -0.576D-03 0.812D-02 0.801D-02 0.524D-01 0.932D-01-0.103D+00

Coeff: -0.147D+00-0.211D-02 0.337D+00 0.754D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=4.73D-07 MaxDP=2.29D-05 DE=-1.34D-08 OVMax= 3.59D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.55D-07 CP: 1.00D+00 1.26D+00 1.34D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.36D+00 1.95D+00 1.01D+00 1.13D+00

E= -1276.01577309377 Delta-E= -0.000000005979 Rises=F Damp=F

DIIS: error= 1.46D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1276.01577309377 IErMin=11 ErrMin= 1.46D-06

ErrMax= 1.46D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.04D-09 BMatP= 8.54D-09

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

Coeff-Com: 0.638D-05-0.408D-02-0.369D-02 0.999D-02 0.437D-01 0.572D-01

Coeff-Com: -0.918D-01-0.174D+00-0.619D-01 0.416D+00 0.808D+00

Coeff: 0.638D-05-0.408D-02-0.369D-02 0.999D-02 0.437D-01 0.572D-01

Coeff: -0.918D-01-0.174D+00-0.619D-01 0.416D+00 0.808D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.29D-07 MaxDP=7.26D-06 DE=-5.98D-09 OVMax= 7.35D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 5.35D-08 CP: 1.00D+00 1.26D+00 1.34D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.38D+00 1.93D+00 9.82D-01 1.36D+00

CP: 1.40D+00

E= -1276.01577309531 Delta-E= -0.000000001543 Rises=F Damp=F

DIIS: error= 8.12D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1276.01577309531 IErMin=12 ErrMin= 8.12D-07

ErrMax= 8.12D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.98D-10 BMatP= 2.04D-09

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

Coeff-Com: 0.121D-03-0.338D-02-0.353D-02-0.590D-02-0.473D-02 0.412D-01

Coeff-Com: -0.110D-02-0.761D-01-0.101D+00 0.393D-01 0.298D+00 0.817D+00

Coeff: 0.121D-03-0.338D-02-0.353D-02-0.590D-02-0.473D-02 0.412D-01

Coeff: -0.110D-02-0.761D-01-0.101D+00 0.393D-01 0.298D+00 0.817D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.01D-07 MaxDP=5.27D-06 DE=-1.54D-09 OVMax= 7.09D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 2.32D-08 CP: 1.00D+00 1.26D+00 1.34D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.39D+00 1.95D+00 1.01D+00 1.47D+00

CP: 1.55D+00 1.18D+00

E= -1276.01577309598 Delta-E= -0.000000000666 Rises=F Damp=F

DIIS: error= 4.16D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1276.01577309598 IErMin=13 ErrMin= 4.16D-07

ErrMax= 4.16D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.83D-10 BMatP= 4.98D-10

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

Coeff-Com: 0.699D-04-0.819D-03-0.140D-02-0.452D-02-0.126D-01 0.700D-02

Coeff-Com: 0.237D-01-0.363D-02-0.477D-01-0.772D-01-0.543D-01 0.439D+00

Coeff-Com: 0.733D+00

Coeff: 0.699D-04-0.819D-03-0.140D-02-0.452D-02-0.126D-01 0.700D-02

Coeff: 0.237D-01-0.363D-02-0.477D-01-0.772D-01-0.543D-01 0.439D+00

Coeff: 0.733D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=4.49D-08 MaxDP=2.80D-06 DE=-6.66D-10 OVMax= 2.96D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 1.47D-08 CP: 1.00D+00 1.26D+00 1.35D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.40D+00 1.96D+00 1.02D+00 1.52D+00

CP: 1.61D+00 1.35D+00 1.20D+00

E= -1276.01577309611 Delta-E= -0.000000000136 Rises=F Damp=F

DIIS: error= 2.36D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1276.01577309611 IErMin=14 ErrMin= 2.36D-07

ErrMax= 2.36D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.52D-11 BMatP= 1.83D-10

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

Coeff-Com: 0.847D-05 0.418D-03 0.227D-04-0.119D-02-0.576D-02-0.811D-02

Coeff-Com: 0.134D-01 0.171D-01-0.281D-02-0.466D-01-0.978D-01 0.312D-01

Coeff-Com: 0.419D+00 0.681D+00

Coeff: 0.847D-05 0.418D-03 0.227D-04-0.119D-02-0.576D-02-0.811D-02

Coeff: 0.134D-01 0.171D-01-0.281D-02-0.466D-01-0.978D-01 0.312D-01

Coeff: 0.419D+00 0.681D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=5.48D-08 MaxDP=2.63D-06 DE=-1.36D-10 OVMax= 4.25D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 5.37D-09 CP: 1.00D+00 1.26D+00 1.35D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.41D+00 1.97D+00 1.03D+00 1.53D+00

CP: 1.62D+00 1.40D+00 1.48D+00 1.05D+00

E= -1276.01577309623 Delta-E= -0.000000000115 Rises=F Damp=F

DIIS: error= 8.72D-08 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1276.01577309623 IErMin=15 ErrMin= 8.72D-08

ErrMax= 8.72D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.73D-12 BMatP= 5.52D-11

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

Coeff-Com: -0.927D-05 0.420D-03 0.284D-03 0.164D-03-0.663D-03-0.695D-02

Coeff-Com: 0.286D-02 0.120D-01 0.824D-02-0.115D-01-0.478D-01-0.831D-01

Coeff-Com: 0.106D+00 0.407D+00 0.613D+00

Coeff: -0.927D-05 0.420D-03 0.284D-03 0.164D-03-0.663D-03-0.695D-02

Coeff: 0.286D-02 0.120D-01 0.824D-02-0.115D-01-0.478D-01-0.831D-01

Coeff: 0.106D+00 0.407D+00 0.613D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=2.42D-08 MaxDP=1.18D-06 DE=-1.15D-10 OVMax= 1.89D-05

Cycle 16 Pass 1 IDiag 1:

RMSU= 1.97D-09 CP: 1.00D+00 1.26D+00 1.35D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.41D+00 1.98D+00 1.04D+00 1.54D+00

CP: 1.62D+00 1.41D+00 1.56D+00 1.19D+00 8.80D-01

E= -1276.01577309619 Delta-E= 0.000000000034 Rises=F Damp=F

DIIS: error= 2.75D-08 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=15 EnMin= -1276.01577309623 IErMin=16 ErrMin= 2.75D-08

ErrMax= 2.75D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.53D-13 BMatP= 9.73D-12

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

Coeff-Com: -0.437D-05 0.918D-04 0.807D-04 0.261D-03 0.684D-03-0.136D-02

Coeff-Com: -0.110D-02 0.214D-02 0.272D-02 0.161D-02-0.456D-02-0.379D-01

Coeff-Com: -0.667D-02 0.733D-01 0.264D+00 0.706D+00

Coeff: -0.437D-05 0.918D-04 0.807D-04 0.261D-03 0.684D-03-0.136D-02

Coeff: -0.110D-02 0.214D-02 0.272D-02 0.161D-02-0.456D-02-0.379D-01

Coeff: -0.667D-02 0.733D-01 0.264D+00 0.706D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.09D-09 MaxDP=8.40D-08 DE= 3.41D-11 OVMax= 4.10D-07

Error on total polarization charges = 0.06995

SCF Done: E(UB3LYP) = -1276.01577310 A.U. after 16 cycles

NFock= 16 Conv=0.11D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7654 S= 0.5077

<L.S>= 0.000000000000E+00

KE= 1.320992333878D+03 PE=-8.598701214197D+03 EE= 3.242157611671D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.67

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7654, after 0.7501

Leave Link 502 at Tue Sep 17 14:03:35 2019, MaxMem= 2415919104 cpu: 1554.2

(Enter /home/blab/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15313 LenP2D= 41232.

LDataN: DoStor=T MaxTD1= 6 Len= 172

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

GePol: Maximum number of non-zero 1st derivatives = 253

Leave Link 701 at Tue Sep 17 14:03:39 2019, MaxMem= 2415919104 cpu: 73.0

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 14:03:39 2019, MaxMem= 2415919104 cpu: 0.3

(Enter /home/blab/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

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

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

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

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

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Tue Sep 17 14:03:51 2019, MaxMem= 2415919104 cpu: 201.6

(Enter /home/blab/g09/l716.exe)

Dipole = 5.25801624D-13 3.64153152D-14-1.33226763D-15

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000812184 -0.000001706 -0.000000000

2 7 -0.001264445 0.001107202 0.000000000

3 6 0.000787296 -0.000545306 0.000000000

4 6 -0.000180741 0.000018875 -0.000000000

5 6 0.000395134 -0.000263314 0.000000000

6 7 -0.000439832 0.000565779 0.000000000

7 6 0.000232679 -0.000798243 -0.000000000

8 7 -0.000446543 0.001447392 0.000000000

9 6 -0.000565271 -0.001112758 -0.000000000

10 6 -0.000060982 0.000368560 -0.000000000

11 6 -0.000159894 -0.000338873 0.000000000

12 7 -0.000357256 -0.000138616 -0.000000000

13 6 0.000060982 -0.000368560 -0.000000000

14 6 0.000159894 0.000338873 -0.000000000

15 6 -0.000232679 0.000798243 0.000000000

16 7 0.000446543 -0.001447392 -0.000000000

17 6 0.000565271 0.001112758 -0.000000000

18 7 0.000439832 -0.000565779 -0.000000000

19 7 0.001264445 -0.001107202 0.000000000

20 6 -0.000787296 0.000545306 -0.000000000

21 6 0.000180741 -0.000018875 -0.000000000

22 6 -0.000395134 0.000263314 -0.000000000

23 6 -0.000812184 0.000001706 0.000000000

24 7 0.000357256 0.000138616 0.000000000

25 30 0.000000000 -0.000000000 0.000000000

26 6 -0.000094183 0.000119125 0.000000000

27 1 0.000056583 -0.000020482 0.000000000

28 6 -0.000141016 -0.000188038 0.000000000

29 1 0.000098098 0.000057758 0.000000000

30 6 0.000141016 0.000188038 -0.000000000

31 1 -0.000098098 -0.000057758 -0.000000000

32 6 0.000094183 -0.000119125 -0.000000000

33 1 -0.000056583 0.000020482 0.000000000

34 1 0.000035137 -0.000089426 0.000000000

35 1 0.000046857 -0.000016956 0.000023165

36 1 0.000046857 -0.000016956 -0.000023165

37 1 0.000015231 0.000064745 0.000023150

38 1 0.000015231 0.000064745 -0.000023150

39 1 0.000041036 0.000033867 0.000000000

40 1 -0.000015231 -0.000064745 0.000023150

41 1 -0.000015231 -0.000064745 -0.000023150

42 1 -0.000041036 -0.000033867 -0.000000000

43 1 -0.000046857 0.000016956 0.000023165

44 1 -0.000046857 0.000016956 -0.000023165

45 1 -0.000035137 0.000089426 -0.000000000

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

Cartesian Forces: Max 0.001447392 RMS 0.000390000

Leave Link 716 at Tue Sep 17 14:03:51 2019, MaxMem= 2415919104 cpu: 0.3

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

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

Internal Forces: Max 0.000705569 RMS 0.000177086

Search for a local minimum.

Step number 8 out of a maximum of 270

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

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4 5

6 7 8

DE= 1.56D-03 DEPred=-2.09D-04 R=-7.49D+00

Trust test=-7.49D+00 RLast= 4.62D-02 DXMaxT set to 1.73D-01

ITU= -1 1 1 1 0 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01329

Eigenvalues --- 0.01330 0.01340 0.01341 0.01609 0.01628

Eigenvalues --- 0.01637 0.01646 0.01771 0.01790 0.01804

Eigenvalues --- 0.01818 0.01886 0.01906 0.01938 0.01948

Eigenvalues --- 0.01997 0.02000 0.02045 0.02048 0.02070

Eigenvalues --- 0.02087 0.02102 0.02110 0.02114 0.02205

Eigenvalues --- 0.02314 0.02317 0.02352 0.02373 0.07166

Eigenvalues --- 0.07187 0.07187 0.07188 0.07188 0.07199

Eigenvalues --- 0.07267 0.07320 0.10409 0.14104 0.14493

Eigenvalues --- 0.14498 0.15544 0.15999 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16011 0.16026

Eigenvalues --- 0.16103 0.16448 0.18720 0.19788 0.22074

Eigenvalues --- 0.22096 0.23571 0.23845 0.23860 0.24252

Eigenvalues --- 0.24369 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25006 0.25060 0.25348

Eigenvalues --- 0.26873 0.27440 0.29439 0.33209 0.33211

Eigenvalues --- 0.33246 0.33282 0.33282 0.33353 0.33629

Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33724 0.33943 0.34312 0.34437

Eigenvalues --- 0.34437 0.34441 0.34449 0.35538 0.35547

Eigenvalues --- 0.35679 0.35682 0.35682 0.35770 0.37213

Eigenvalues --- 0.38700 0.41598 0.41774 0.41865 0.43963

Eigenvalues --- 0.47981 0.48965 0.48984 0.50971 0.51361

Eigenvalues --- 0.51363 0.51879 0.53077 0.53841 0.54013

Eigenvalues --- 0.54028 0.56327 0.56337 0.56704

Cosine: -0.051 < 0.620

Cut down GDIIS permanently because of the cosine check. E 8

DIIS coeff's: 0.97978 0.13139 -0.06634 0.11677 -0.16161

Cosine: 0.991 > 0.670

Length: 0.830

GDIIS step was calculated using 5 of the last 8 vectors.

Iteration 1 RMS(Cart)= 0.00129275 RMS(Int)= 0.00000277

Iteration 2 RMS(Cart)= 0.00000203 RMS(Int)= 0.00000261

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000261

ITry= 1 IFail=0 DXMaxC= 4.34D-03 DCOld= 1.00D+10 DXMaxT= 1.73D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 8.35D-11 for atom 12.

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

(Linear) (Quad) (Total)

R1 2.58568 -0.00071 -0.00245 -0.00088 -0.00333 2.58236

R2 2.71132 0.00034 0.00095 -0.00003 0.00092 2.71223

R3 2.58180 0.00020 0.00086 0.00086 0.00172 2.58352

R4 2.58024 0.00056 0.00202 0.00061 0.00263 2.58287

R5 3.80553 -0.00042 -0.00074 -0.00041 -0.00115 3.80438

R6 2.72887 -0.00019 -0.00027 -0.00110 -0.00136 2.72750

R7 2.58171 -0.00064 -0.00134 -0.00058 -0.00191 2.57981

R8 2.62495 -0.00033 -0.00001 -0.00033 -0.00033 2.62462

R9 2.82504 0.00001 -0.00001 0.00032 0.00031 2.82535

R10 2.04565 -0.00004 -0.00006 -0.00008 -0.00014 2.04551

R11 2.50270 -0.00054 -0.00195 -0.00046 -0.00240 2.50030

R12 2.58536 0.00050 0.00192 0.00076 0.00268 2.58804

R13 2.77864 -0.00013 0.00014 -0.00041 -0.00027 2.77837

R14 2.58787 -0.00063 -0.00231 -0.00115 -0.00347 2.58440

R15 3.79622 -0.00066 -0.00083 -0.00136 -0.00220 3.79402

R16 2.80344 -0.00018 0.00208 -0.00132 0.00076 2.80420

R17 2.49529 0.00034 0.00059 0.00046 0.00106 2.49634

R18 2.56752 0.00007 -0.00056 0.00019 -0.00036 2.56716

R19 2.81645 -0.00008 0.00016 -0.00048 -0.00032 2.81614

R20 2.04512 0.00000 -0.00008 0.00012 0.00004 2.04516

R21 2.49529 0.00034 0.00059 0.00046 0.00106 2.49634

R22 2.56752 0.00007 -0.00056 0.00019 -0.00036 2.56716

R23 2.80344 -0.00018 0.00208 -0.00132 0.00076 2.80420

R24 2.81645 -0.00008 0.00016 -0.00048 -0.00032 2.81614

R25 2.77864 -0.00013 0.00014 -0.00041 -0.00027 2.77837

R26 2.04512 0.00000 -0.00008 0.00012 0.00004 2.04516

R27 2.58536 0.00050 0.00192 0.00076 0.00268 2.58804

R28 2.50270 -0.00054 -0.00195 -0.00046 -0.00240 2.50030

R29 2.58787 -0.00063 -0.00231 -0.00115 -0.00347 2.58440

R30 3.79622 -0.00066 -0.00083 -0.00136 -0.00220 3.79402

R31 2.58171 -0.00064 -0.00134 -0.00058 -0.00191 2.57981

R32 2.58024 0.00056 0.00202 0.00061 0.00263 2.58287

R33 2.58568 -0.00071 -0.00245 -0.00088 -0.00333 2.58236

R34 3.80553 -0.00042 -0.00074 -0.00041 -0.00115 3.80438

R35 2.72887 -0.00019 -0.00027 -0.00110 -0.00136 2.72750

R36 2.62495 -0.00033 -0.00001 -0.00033 -0.00033 2.62462

R37 2.82504 0.00001 -0.00001 0.00032 0.00031 2.82535

R38 2.71132 0.00034 0.00095 -0.00003 0.00092 2.71223

R39 2.04565 -0.00004 -0.00006 -0.00008 -0.00014 2.04551

R40 2.58180 0.00020 0.00086 0.00086 0.00172 2.58352

R41 2.06449 0.00003 -0.00005 0.00007 0.00002 2.06451

R42 2.07007 0.00005 0.00015 -0.00012 0.00003 2.07009

R43 2.07007 0.00005 0.00015 -0.00012 0.00003 2.07009

R44 2.06883 0.00006 0.00024 -0.00019 0.00005 2.06888

R45 2.06883 0.00006 0.00024 -0.00019 0.00005 2.06888

R46 2.06320 0.00000 0.00004 -0.00003 0.00001 2.06321

R47 2.06883 0.00006 0.00024 -0.00019 0.00005 2.06888

R48 2.06883 0.00006 0.00024 -0.00019 0.00005 2.06888

R49 2.06320 0.00000 0.00004 -0.00003 0.00001 2.06321

R50 2.07007 0.00005 0.00015 -0.00012 0.00003 2.07009

R51 2.07007 0.00005 0.00015 -0.00012 0.00003 2.07009

R52 2.06449 0.00003 -0.00005 0.00007 0.00002 2.06451

A1 1.88800 0.00005 0.00077 -0.00033 0.00043 1.88843

A2 2.20724 -0.00024 0.00088 -0.00084 0.00004 2.20728

A3 2.18794 0.00019 -0.00165 0.00117 -0.00047 2.18747

A4 1.90604 -0.00013 -0.00027 0.00007 -0.00019 1.90584

A5 2.18803 0.00045 0.00060 0.00156 0.00215 2.19018

A6 2.18912 -0.00032 -0.00033 -0.00163 -0.00196 2.18716

A7 1.89737 0.00009 -0.00013 0.00005 -0.00008 1.89728

A8 2.21442 0.00008 -0.00075 0.00047 -0.00028 2.21414

A9 2.17140 -0.00017 0.00089 -0.00052 0.00037 2.17177

A10 1.85398 -0.00012 -0.00000 -0.00015 -0.00015 1.85383

A11 2.18835 -0.00006 0.00046 -0.00058 -0.00012 2.18823

A12 2.24086 0.00018 -0.00046 0.00073 0.00027 2.24112

A13 1.87940 0.00011 -0.00037 0.00036 -0.00001 1.87939

A14 2.18523 -0.00001 0.00004 -0.00002 0.00002 2.18525

A15 2.21856 -0.00010 0.00033 -0.00034 -0.00001 2.21855

A16 2.17481 0.00023 0.00124 0.00111 0.00235 2.17716

A17 2.23035 -0.00016 0.00007 -0.00096 -0.00089 2.22946

A18 2.17370 0.00005 0.00089 -0.00006 0.00083 2.17454

A19 1.87913 0.00011 -0.00097 0.00102 0.00006 1.87919

A20 1.91447 -0.00021 0.00062 -0.00130 -0.00068 1.91378

A21 2.19002 -0.00004 -0.00087 -0.00027 -0.00114 2.18888

A22 2.17870 0.00026 0.00026 0.00157 0.00182 2.18052

A23 1.88480 0.00026 0.00016 0.00102 0.00117 1.88598

A24 2.23813 0.00001 0.00135 -0.00035 0.00101 2.23914

A25 2.16025 -0.00027 -0.00152 -0.00067 -0.00218 2.15807

A26 1.85873 0.00007 -0.00060 0.00040 -0.00019 1.85854

A27 2.16565 -0.00007 -0.00091 0.00014 -0.00077 2.16488

A28 2.25880 0.00000 0.00151 -0.00054 0.00097 2.25977

A29 1.88764 -0.00023 0.00079 -0.00114 -0.00035 1.88729

A30 2.16875 0.00023 -0.00102 0.00136 0.00033 2.16909

A31 2.22679 -0.00000 0.00024 -0.00022 0.00002 2.22680

A32 2.18032 -0.00026 -0.00244 -0.00066 -0.00309 2.17723

A33 1.85873 0.00007 -0.00060 0.00040 -0.00019 1.85854

A34 2.25880 0.00000 0.00151 -0.00054 0.00097 2.25977

A35 2.16565 -0.00007 -0.00091 0.00014 -0.00077 2.16488

A36 1.88764 -0.00023 0.00079 -0.00114 -0.00035 1.88729

A37 2.22679 -0.00000 0.00024 -0.00022 0.00002 2.22680

A38 2.16875 0.00023 -0.00102 0.00136 0.00033 2.16909

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A40 2.17370 0.00005 0.00089 -0.00006 0.00083 2.17454

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A42 1.91447 -0.00021 0.00062 -0.00130 -0.00068 1.91378

A43 2.19002 -0.00004 -0.00087 -0.00027 -0.00114 2.18888

A44 2.17870 0.00026 0.00026 0.00157 0.00182 2.18052

A45 2.16025 -0.00027 -0.00152 -0.00067 -0.00218 2.15807

A46 2.23813 0.00001 0.00135 -0.00035 0.00101 2.23914

A47 1.88480 0.00026 0.00016 0.00102 0.00117 1.88598

A48 2.17481 0.00023 0.00124 0.00111 0.00235 2.17716

A49 1.90604 -0.00013 -0.00027 0.00007 -0.00019 1.90584

A50 2.18912 -0.00032 -0.00033 -0.00163 -0.00196 2.18716

A51 2.18803 0.00045 0.00060 0.00156 0.00215 2.19018

A52 2.21442 0.00008 -0.00075 0.00047 -0.00028 2.21414

A53 2.17140 -0.00017 0.00089 -0.00052 0.00037 2.17177

A54 1.89737 0.00009 -0.00013 0.00005 -0.00008 1.89728

A55 1.85398 -0.00012 -0.00000 -0.00015 -0.00015 1.85383

A56 2.18835 -0.00006 0.00046 -0.00058 -0.00012 2.18823

A57 2.24086 0.00018 -0.00046 0.00073 0.00027 2.24112

A58 1.87940 0.00011 -0.00037 0.00036 -0.00001 1.87939

A59 2.21856 -0.00010 0.00033 -0.00034 -0.00001 2.21855

A60 2.18523 -0.00001 0.00004 -0.00002 0.00002 2.18525

A61 1.88800 0.00005 0.00077 -0.00033 0.00043 1.88843

A62 2.20724 -0.00024 0.00088 -0.00084 0.00004 2.20728

A63 2.18794 0.00019 -0.00165 0.00117 -0.00047 2.18747

A64 2.18032 -0.00026 -0.00244 -0.00066 -0.00309 2.17723

A65 1.56765 0.00021 0.00065 0.00128 0.00193 1.56957

A66 1.57395 -0.00021 -0.00065 -0.00128 -0.00193 1.57202

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A69 1.94082 0.00014 -0.00065 0.00125 0.00059 1.94141

A70 1.94990 -0.00001 -0.00030 0.00020 -0.00010 1.94979

A71 1.94990 -0.00001 -0.00030 0.00020 -0.00010 1.94979

A72 1.88081 -0.00005 0.00032 -0.00041 -0.00009 1.88072

A73 1.88081 -0.00005 0.00032 -0.00041 -0.00009 1.88072

A74 1.85753 -0.00003 0.00073 -0.00097 -0.00023 1.85729

A75 1.93977 -0.00000 -0.00025 0.00001 -0.00024 1.93953

A76 1.93977 -0.00000 -0.00025 0.00001 -0.00024 1.93953

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A78 1.85811 -0.00004 0.00038 -0.00072 -0.00033 1.85777

A79 1.88910 -0.00002 0.00021 -0.00016 0.00005 1.88915

A80 1.88910 -0.00002 0.00021 -0.00016 0.00005 1.88915

A81 1.93977 -0.00000 -0.00025 0.00001 -0.00024 1.93953

A82 1.93977 -0.00000 -0.00025 0.00001 -0.00024 1.93953

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A86 1.88910 -0.00002 0.00021 -0.00016 0.00005 1.88915

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A89 1.94082 0.00014 -0.00065 0.00125 0.00059 1.94141

A90 1.85753 -0.00003 0.00073 -0.00097 -0.00023 1.85729

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D31 -1.03938 0.00003 -0.00026 0.00048 0.00022 -1.03916

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D45 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D63 1.03303 -0.00003 0.00008 -0.00044 -0.00036 1.03267

D64 -1.03303 0.00003 -0.00008 0.00044 0.00036 -1.03267

D65 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D66 -2.10856 -0.00003 0.00008 -0.00044 -0.00036 -2.10893

D67 2.10856 0.00003 -0.00008 0.00044 0.00036 2.10893

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D79 -2.10856 -0.00003 0.00008 -0.00044 -0.00036 -2.10893

D80 2.10856 0.00003 -0.00008 0.00044 0.00036 2.10893

D81 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D82 1.03303 -0.00003 0.00008 -0.00044 -0.00036 1.03267

D83 -1.03303 0.00003 -0.00008 0.00044 0.00036 -1.03267

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D125 1.03938 -0.00003 0.00026 -0.00048 -0.00022 1.03916

D126 -1.03938 0.00003 -0.00026 0.00048 0.00022 -1.03916

D127 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D128 -2.10221 -0.00003 0.00026 -0.00048 -0.00022 -2.10243

D129 2.10221 0.00003 -0.00026 0.00048 0.00022 2.10243

D130 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

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D134 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

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D136 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

Item Value Threshold Converged?

Maximum Force 0.000706 0.000450 NO

RMS Force 0.000177 0.000300 YES

Maximum Displacement 0.004341 0.001800 NO

RMS Displacement 0.001294 0.001200 NO

Predicted change in Energy=-2.207332D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:03:51 2019, MaxMem= 2415919104 cpu: 1.7

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.073513 -2.194322 -0.000000

2 7 0 -0.746072 -1.869843 -0.000000

3 6 0 -0.003007 -3.017004 -0.000000

4 6 0 -0.898758 -4.148745 -0.000000

5 6 0 -2.185200 -3.625223 -0.000000

6 7 0 1.358962 -3.110521 -0.000000

7 6 0 2.185678 -2.077497 -0.000000

8 7 0 1.863841 -0.746319 -0.000000

9 6 0 3.007643 0.003392 -0.000000

10 6 0 4.165764 -0.924387 -0.000000

11 6 0 3.652206 -2.182057 -0.000000

12 7 0 -3.123924 -1.319272 -0.000000

13 6 0 -4.165764 0.924387 -0.000000

14 6 0 -3.652206 2.182057 -0.000000

15 6 0 -2.185678 2.077497 -0.000000

16 7 0 -1.863841 0.746319 -0.000000

17 6 0 -3.007643 -0.003392 -0.000000

18 7 0 -1.358962 3.110521 -0.000000

19 7 0 0.746072 1.869843 -0.000000

20 6 0 0.003007 3.017004 -0.000000

21 6 0 0.898758 4.148745 -0.000000

22 6 0 2.185200 3.625223 -0.000000

23 6 0 2.073513 2.194322 -0.000000

24 7 0 3.123924 1.319272 -0.000000

25 30 0 0.000000 -0.000000 -0.000000

26 6 0 -0.480061 -5.584031 -0.000000

27 1 0 -3.115529 -4.178544 -0.000000

28 6 0 5.588867 -0.482147 -0.000000

29 1 0 4.196625 -3.117407 -0.000000

30 6 0 -5.588867 0.482147 -0.000000

31 1 0 -4.196625 3.117407 -0.000000

32 6 0 0.480061 5.584031 -0.000000

33 1 0 3.115529 4.178544 -0.000000

34 1 0 -1.346819 -6.249063 -0.000000

35 1 0 0.128720 -5.828635 0.877245

36 1 0 0.128720 -5.828635 -0.877245

37 1 0 5.810372 0.134781 0.876887

38 1 0 5.810372 0.134781 -0.876887

39 1 0 6.271959 -1.333865 -0.000000

40 1 0 -5.810372 -0.134781 0.876887

41 1 0 -5.810372 -0.134781 -0.876887

42 1 0 -6.271959 1.333865 -0.000000

43 1 0 -0.128720 5.828635 0.877245

44 1 0 -0.128720 5.828635 -0.877245

45 1 0 1.346819 6.249063 -0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.366524 0.000000

3 C 2.227959 1.366794 0.000000

4 C 2.280311 2.284011 1.443332 0.000000

5 C 1.435253 2.269901 2.265369 1.388888 0.000000

6 N 3.552648 2.443450 1.365176 2.484997 3.581341

7 C 4.260793 2.939094 2.381809 3.715348 4.636812

8 N 4.195173 2.841470 2.939581 4.382745 4.968181

9 C 5.536072 4.195162 4.264599 5.700896 6.335019

10 C 6.367206 5.002001 4.664514 6.003821 6.901395

11 C 5.725733 4.409346 3.749363 4.957735 6.013156

12 N 1.367142 2.440760 3.552805 3.599623 2.489701

13 C 3.755511 4.416108 5.732636 6.034070 4.962014

14 C 4.652415 4.986332 6.351921 6.903661 5.989709

15 C 4.273292 4.201661 5.542382 6.357850 5.702720

16 N 2.948106 2.844945 4.198250 4.989292 4.383338

17 C 2.381758 2.932292 4.255548 4.650951 3.714037

18 N 5.352751 5.017934 6.275761 7.273839 6.786230

19 N 4.946463 4.026381 4.943925 6.239300 6.228010

20 C 5.609800 4.943925 6.034012 7.222267 6.993385

21 C 7.004920 6.239300 7.222267 8.489959 8.363335

22 C 7.211362 6.228010 6.993385 8.363335 8.465776

23 C 6.038048 4.946463 5.609800 7.004920 7.211362

24 N 6.273651 5.014711 5.346119 6.788312 7.254987

25 Zn 3.019024 2.013191 3.017006 4.244980 4.232888

26 C 3.745560 3.723702 2.610978 1.495110 2.597004

27 H 2.241190 3.308236 3.322193 2.216972 1.082440

28 C 7.851345 6.485149 6.139589 7.452061 8.385407

29 H 6.337722 5.097712 4.200831 5.198709 6.401997

30 C 4.418281 5.383728 6.591350 6.591077 5.334364

31 H 5.720321 6.064567 7.430844 7.979530 7.036256

32 C 8.186790 7.554048 8.614590 9.829958 9.587178

33 H 8.218247 7.175998 7.842269 9.244362 9.433796

34 H 4.119346 4.420234 3.500291 2.147579 2.754527

35 H 4.339080 4.148114 2.948250 2.155759 3.313428

36 H 4.339080 4.148114 2.948250 2.155759 3.313428

37 H 8.267364 6.911904 6.670687 8.008118 8.878950

38 H 8.267364 6.911904 6.670687 8.008118 8.878950

39 H 8.389714 7.038468 6.496780 7.703423 8.762069

40 H 4.356002 5.424621 6.542296 6.403499 5.108228

41 H 4.356002 5.424621 6.542296 6.403499 5.108228

42 H 5.484073 6.387423 7.630847 7.676608 6.426053

43 H 8.301784 7.772853 8.889921 10.045428 9.714633

44 H 8.301784 7.772853 8.889921 10.045428 9.714633

45 H 9.109853 8.384320 9.363869 10.637529 10.486977

6 7 8 9 10

6 N 0.000000

7 C 1.323101 0.000000

8 N 2.417510 1.369531 0.000000

9 C 3.523436 2.237348 1.367607 0.000000

10 C 3.557712 2.291376 2.308800 1.483920 0.000000

11 C 2.474068 1.470252 2.293381 2.278520 1.358483

12 N 4.827509 5.363467 5.020565 6.272603 7.300376

13 C 6.841277 7.025106 6.256788 7.232288 8.534185

14 C 7.288566 7.226665 6.245171 7.007151 8.412530

15 C 6.283311 6.030980 4.936855 5.592181 7.025106

16 N 5.026099 4.936855 4.015418 4.927808 6.256788

17 C 5.359243 5.592181 4.927808 6.015289 7.232288

18 N 6.788849 6.283311 5.026099 5.359243 6.841277

19 N 5.017934 4.201661 2.844945 2.932292 4.416108

20 C 6.275761 5.542382 4.198250 4.255548 5.732636

21 C 7.273839 6.357850 4.989292 4.650951 6.034070

22 C 6.786230 5.702720 4.383338 3.714037 4.962014

23 C 5.352751 4.273292 2.948106 2.381758 3.755511

24 N 4.768454 3.523967 2.419602 1.321007 2.473749

25 Zn 3.394424 3.015490 2.007709 3.007645 4.267093

26 C 3.082249 4.404764 5.375625 6.586606 6.579967

27 H 4.600189 5.702385 6.047669 7.414973 7.975385

28 C 4.980005 3.758569 3.734382 2.626494 1.490235

29 H 2.837671 2.263917 3.326250 3.339621 2.193237

30 C 7.821739 8.185067 7.553277 8.609831 9.855514

31 H 8.345755 8.229266 7.187324 7.848475 9.287930

32 C 8.738862 7.849086 6.479829 6.126353 7.479567

33 H 7.497732 6.324766 5.081436 4.176545 5.209884

34 H 4.143875 5.466305 6.370913 7.619353 7.664251

35 H 3.109855 4.367112 5.441520 6.562796 6.412404

36 H 3.109855 4.367112 5.441520 6.562796 6.412404

37 H 5.578169 4.336072 4.137678 2.939641 2.143713

38 H 5.578169 4.336072 4.137678 2.939641 2.143713

39 H 5.224370 4.153394 4.447102 3.527608 2.145631

40 H 7.811742 8.275258 7.748320 8.862585 10.045681

41 H 7.811742 8.275258 7.748320 8.862585 10.045681

42 H 8.830828 9.119704 8.397524 9.374496 10.679221

43 H 9.104464 8.284498 6.926028 6.673813 8.050804

44 H 9.104464 8.284498 6.926028 6.673813 8.050804

45 H 9.359592 8.368709 7.014462 6.462719 7.707454

11 12 13 14 15

11 C 0.000000

12 N 6.830838 0.000000

13 C 8.412530 2.473749 0.000000

14 C 8.508815 3.540959 1.358483 0.000000

15 C 7.226665 3.523967 2.291376 1.470252 0.000000

16 N 6.245171 2.419602 2.308800 2.293381 1.369531

17 C 7.007151 1.321007 1.483920 2.278520 2.237348

18 N 7.288566 4.768454 3.557712 2.474068 1.323101

19 N 4.986332 5.014711 5.002001 4.409346 2.939094

20 C 6.351921 5.346119 4.664514 3.749363 2.381809

21 C 6.903661 6.788312 6.003821 4.957735 3.715348

22 C 5.989709 7.254987 6.901395 6.013156 4.636812

23 C 4.652415 6.273651 6.367206 5.725733 4.260793

24 N 3.540959 6.782147 7.300376 6.830838 5.363467

25 Zn 4.254408 3.391074 4.267093 4.254408 3.015490

26 C 5.352481 5.017787 7.479567 8.388959 7.849086

27 H 7.056076 2.859284 5.209884 6.383202 6.324766

28 C 2.576887 8.752914 9.855514 9.617454 8.185067

29 H 1.082253 7.538151 9.287930 9.470400 8.229266

30 C 9.617454 3.053040 1.490235 2.576887 3.758569

31 H 9.470400 4.564516 2.193237 1.082253 2.263917

32 C 8.388959 7.787445 6.579967 5.352481 4.404764

33 H 6.383202 8.316054 7.975385 7.056076 5.702385

34 H 6.444439 5.240319 7.707454 8.740630 8.368709

35 H 5.146071 5.628819 8.050804 8.901469 8.284498

36 H 5.146071 5.628819 8.050804 8.901469 8.284498

37 H 3.285476 9.094221 10.045681 9.721145 8.275258

38 H 3.285476 9.094221 10.045681 9.721145 8.275258

39 H 2.753640 9.395895 10.679221 10.528569 9.119704

40 H 9.721145 3.064140 2.143713 3.285476 4.336072

41 H 9.721145 3.064140 2.143713 3.285476 4.336072

42 H 10.528569 4.116948 2.145631 2.753640 4.153394

43 H 8.901469 7.799576 6.412404 5.146071 4.367112

44 H 8.901469 7.799576 6.412404 5.146071 4.367112

45 H 8.740630 8.790179 7.664251 6.444439 5.466305

16 17 18 19 20

16 N 0.000000

17 C 1.367607 0.000000

18 N 2.417510 3.523436 0.000000

19 N 2.841470 4.195162 2.443450 0.000000

20 C 2.939581 4.264599 1.365176 1.366794 0.000000

21 C 4.382745 5.700896 2.484997 2.284011 1.443332

22 C 4.968181 6.335019 3.581341 2.269901 2.265369

23 C 4.195173 5.536072 3.552648 1.366524 2.227959

24 N 5.020565 6.272603 4.827509 2.440760 3.552805

25 Zn 2.007709 3.007645 3.394424 2.013191 3.017006

26 C 6.479829 6.126353 8.738862 7.554048 8.614590

27 H 5.081436 4.176545 7.497732 7.175998 7.842269

28 C 7.553277 8.609831 7.821739 5.383728 6.591350

29 H 7.187324 7.848475 8.345755 6.064567 7.430844

30 C 3.734382 2.626494 4.980005 6.485149 6.139589

31 H 3.326250 3.339621 2.837671 5.097712 4.200831

32 C 5.375625 6.586606 3.082249 3.723702 2.610978

33 H 6.047669 7.414973 4.600189 3.308236 3.322193

34 H 7.014462 6.462719 9.359592 8.384320 9.363869

35 H 6.926028 6.673813 9.104464 7.772853 8.889921

36 H 6.926028 6.673813 9.104464 7.772853 8.889921

37 H 7.748320 8.862585 7.811742 5.424621 6.542296

38 H 7.748320 8.862585 7.811742 5.424621 6.542296

39 H 8.397524 9.374496 8.830828 6.387423 7.630847

40 H 4.137678 2.939641 5.578169 6.911904 6.670687

41 H 4.137678 2.939641 5.578169 6.911904 6.670687

42 H 4.447102 3.527608 5.224370 7.038468 6.496780

43 H 5.441520 6.562796 3.109855 4.148114 2.948250

44 H 5.441520 6.562796 3.109855 4.148114 2.948250

45 H 6.370913 7.619353 4.143875 4.420234 3.500291

21 22 23 24 25

21 C 0.000000

22 C 1.388888 0.000000

23 C 2.280311 1.435253 0.000000

24 N 3.599623 2.489701 1.367142 0.000000

25 Zn 4.244980 4.232888 3.019024 3.391074 0.000000

26 C 9.829958 9.587178 8.186790 7.787445 5.604629

27 H 9.244362 9.433796 8.218247 8.316054 5.212173

28 C 6.591077 5.334364 4.418281 3.053040 5.609626

29 H 7.979530 7.036256 5.720321 4.564516 5.227799

30 C 7.452061 8.385407 7.851345 8.752914 5.609626

31 H 5.198709 6.401997 6.337722 7.538151 5.227799

32 C 1.495110 2.597004 3.745560 5.017787 5.604629

33 H 2.216972 1.082440 2.241190 2.859284 5.212173

34 H 10.637529 10.486977 9.109853 8.790179 6.392551

35 H 10.045428 9.714633 8.301784 7.799576 5.895686

36 H 10.045428 9.714633 8.301784 7.799576 5.895686

37 H 6.403499 5.108228 4.356002 3.064140 5.877714

38 H 6.403499 5.108228 4.356002 3.064140 5.877714

39 H 7.676608 6.426053 5.484073 4.116948 6.412228

40 H 8.008118 8.878950 8.267364 9.094221 5.877714

41 H 8.008118 8.878950 8.267364 9.094221 5.877714

42 H 7.703423 8.762069 8.389714 9.395895 6.412228

43 H 2.155759 3.313428 4.339080 5.628819 5.895686

44 H 2.155759 3.313428 4.339080 5.628819 5.895686

45 H 2.147579 2.754527 4.119346 5.240319 6.392551

26 27 28 29 30

26 C 0.000000

27 H 2.986819 0.000000

28 C 7.928500 9.456736 0.000000

29 H 5.287307 7.388748 2.980425 0.000000

30 C 7.930853 5.276309 11.219252 10.426536 0.000000

31 H 9.461918 7.375613 10.426536 10.455599 2.980425

32 C 11.209258 10.403660 7.930853 9.461918 7.928500

33 H 10.403660 10.424346 5.276309 7.375613 9.456736

34 H 1.092491 2.723121 9.020036 6.366870 7.956392

35 H 1.095446 3.743996 7.692054 4.966705 8.560743

36 H 1.095446 3.743996 7.692054 4.966705 8.560743

37 H 8.546537 9.952157 1.094804 3.734949 11.438193

38 H 8.546537 9.952157 1.094804 3.734949 11.438193

39 H 7.978326 9.809033 1.091805 2.736428 11.999046

40 H 7.673036 4.937927 11.438193 10.478787 1.094804

41 H 7.673036 4.937927 11.438193 10.478787 1.094804

42 H 9.022382 6.352141 11.999046 11.375635 1.091805

43 H 11.451722 10.480182 8.560743 9.975461 7.692054

44 H 11.451722 10.480182 8.560743 9.975461 7.692054

45 H 11.973288 11.342290 7.956392 9.790412 9.020036

31 32 33 34 35

31 H 0.000000

32 C 5.287307 0.000000

33 H 7.388748 2.986819 0.000000

34 H 9.790412 11.973288 11.342290 0.000000

35 H 9.975461 11.451722 10.480182 1.767352 0.000000

36 H 9.975461 11.451722 10.480182 1.767352 1.754489

37 H 10.478787 7.673036 4.937927 9.630565 8.236717

38 H 10.478787 7.673036 4.937927 9.630565 8.421430

39 H 11.375635 9.022382 6.352141 9.066694 7.662369

40 H 3.734949 8.546537 9.952157 7.620806 8.227562

41 H 3.734949 8.546537 9.952157 7.620806 8.412476

42 H 2.736428 7.978326 9.809033 9.042003 9.645706

43 H 4.966705 1.095446 3.743996 12.170625 11.660112

44 H 4.966705 1.095446 3.743996 12.170625 11.791371

45 H 6.366870 1.092491 2.723121 12.785103 12.170625

36 37 38 39 40

36 H 0.000000

37 H 8.421430 0.000000

38 H 8.236717 1.753774 0.000000

39 H 7.662369 1.771699 1.771699 0.000000

40 H 8.412476 11.623871 11.755429 12.173310 0.000000

41 H 8.227562 11.755429 11.623871 12.173310 1.753774

42 H 9.645706 12.173310 12.173310 12.824456 1.771699

43 H 11.791371 8.227562 8.412476 9.645706 8.236717

44 H 11.660112 8.412476 8.227562 9.645706 8.421430

45 H 12.170625 7.620806 7.620806 9.042003 9.630565

41 42 43 44 45

41 H 0.000000

42 H 1.771699 0.000000

43 H 8.421430 7.662369 0.000000

44 H 8.236717 7.662369 1.754489 0.000000

45 H 9.630565 9.066694 1.767352 1.767352 0.000000

Stoichiometry C20H16N8Zn(1-,2)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=3 Diff= 4.81D-04

Largest Abelian subgroup C2H NOp 4

Largest concise Abelian subgroup C2H NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.947212 0.654559 0.000000

2 7 0 -1.987826 -0.318563 0.000000

3 6 0 -2.591497 -1.544820 0.000000

4 6 0 -4.022467 -1.356323 0.000000

5 6 0 -4.232856 0.016538 0.000000

6 7 0 -1.973231 -2.761969 0.000000

7 6 0 -0.662413 -2.941834 0.000000

8 7 0 0.315273 -1.982801 0.000000

9 6 0 1.545512 -2.580178 0.000000

10 6 0 1.343050 -4.050222 0.000000

11 6 0 0.000000 -4.254408 0.000000

12 7 0 -2.734772 2.005094 0.000000

13 6 0 -1.343050 4.050222 0.000000

14 6 0 0.000000 4.254408 0.000000

15 6 0 0.662413 2.941834 0.000000

16 7 0 -0.315273 1.982801 0.000000

17 6 0 -1.545512 2.580178 0.000000

18 7 0 1.973231 2.761969 0.000000

19 7 0 1.987826 0.318563 0.000000

20 6 0 2.591497 1.544820 0.000000

21 6 0 4.022467 1.356323 0.000000

22 6 0 4.232856 -0.016538 0.000000

23 6 0 2.947212 -0.654559 0.000000

24 7 0 2.734772 -2.005094 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -5.039845 -2.451903 0.000000

27 1 0 -5.185015 0.531386 0.000000

28 6 0 2.452592 -5.045066 0.000000

29 1 0 -0.523725 -5.201500 0.000000

30 6 0 -2.452592 5.045066 0.000000

31 1 0 0.523725 5.201500 0.000000

32 6 0 5.039845 2.451903 0.000000

33 1 0 5.185015 -0.531386 0.000000

34 1 0 -6.055297 -2.048923 0.000000

35 1 0 -4.937586 -3.099967 0.877245

36 1 0 -4.937586 -3.099967 -0.877245

37 1 0 3.095805 -4.918799 0.876887

38 1 0 3.095805 -4.918799 -0.876887

39 1 0 2.071786 -6.068309 0.000000

40 1 0 -3.095805 4.918799 0.876887

41 1 0 -3.095805 4.918799 -0.876887

42 1 0 -2.071786 6.068309 0.000000

43 1 0 4.937586 3.099967 0.877245

44 1 0 4.937586 3.099967 -0.877245

45 1 0 6.055297 2.048923 0.000000

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

Rotational constants (GHZ): 0.1827567 0.1816562 0.0913066

Leave Link 202 at Tue Sep 17 14:03:51 2019, MaxMem= 2415919104 cpu: 0.2

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 229 symmetry adapted cartesian basis functions of AG symmetry.

There are 82 symmetry adapted cartesian basis functions of BG symmetry.

There are 78 symmetry adapted cartesian basis functions of AU symmetry.

There are 218 symmetry adapted cartesian basis functions of BU symmetry.

There are 212 symmetry adapted basis functions of AG symmetry.

There are 82 symmetry adapted basis functions of BG symmetry.

There are 78 symmetry adapted basis functions of AU symmetry.

There are 204 symmetry adapted basis functions of BU symmetry.

576 basis functions, 1015 primitive gaussians, 607 cartesian basis functions

103 alpha electrons 102 beta electrons

nuclear repulsion energy 2760.1818433229 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= 45 NActive= 45 NUniq= 21 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1141509631 Hartrees.

Nuclear repulsion after empirical dispersion term = 2760.0676923598 Hartrees.

No density basis found on file 724.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

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 = 45

GePol: Total number of spheres = 45

GePol: Number of exposed spheres = 45 (100.00%)

GePol: Number of points = 3616

GePol: Average weight of points = 0.10

GePol: Minimum weight of points = 0.24D-09

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 280

GePol: Fraction of low-weight points (<1% of avg) = 7.74%

GePol: Cavity surface area = 378.867 Ang\*\*2

GePol: Cavity volume = 378.233 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0106430218 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2760.0570493380 Hartrees.

Leave Link 301 at Tue Sep 17 14:03:51 2019, MaxMem= 2415919104 cpu: 2.2

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15317 LenP2D= 41234.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.79D-04 NBF= 212 82 78 204

NBsUse= 576 1.00D-06 EigRej= -1.00D+00 NBFU= 212 82 78 204

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= 594 594 594 594 594 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Tue Sep 17 14:03:52 2019, MaxMem= 2415919104 cpu: 13.0

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:03:52 2019, MaxMem= 2415919104 cpu: 1.3

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

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

B after Tr= -0.000000 -0.000000 -0.000000

Rot= 1.000000 -0.000000 0.000000 -0.000119 Ang= -0.01 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

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

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7654 S= 0.5076

Leave Link 401 at Tue Sep 17 14:03:53 2019, MaxMem= 2415919104 cpu: 20.4

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1141655 IEndB= 1141655 NGot= 2415919104 MDV= 2415163146

LenX= 2415163146 LenY= 2414794090

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= 670000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 39226368.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.99D-15 for 3603.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.93D-15 for 1959 731.

Iteration 1 A^-1\*A deviation from unit magnitude is 8.44D-15 for 3603.

Iteration 1 A^-1\*A deviation from orthogonality is 3.14D-12 for 1975 1971.

E= -1276.01576222781

DIIS: error= 1.54D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1276.01576222781 IErMin= 1 ErrMin= 1.54D-04

ErrMax= 1.54D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.14D-05 BMatP= 8.14D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.54D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.294 Goal= None Shift= 0.000

Gap= 0.342 Goal= None Shift= 0.000

RMSDP=1.43D-05 MaxDP=3.60D-04 OVMax= 4.11D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.43D-05 CP: 1.00D+00

E= -1276.01578922796 Delta-E= -0.000027000156 Rises=F Damp=F

DIIS: error= 1.35D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1276.01578922796 IErMin= 2 ErrMin= 1.35D-04

ErrMax= 1.35D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.04D-05 BMatP= 8.14D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.35D-03

Coeff-Com: 0.138D+00 0.862D+00

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

Coeff: 0.138D+00 0.862D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=7.71D-06 MaxDP=3.72D-04 DE=-2.70D-05 OVMax= 4.60D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 7.66D-06 CP: 1.00D+00 1.06D+00

E= -1276.01578701576 Delta-E= 0.000002212202 Rises=F Damp=F

DIIS: error= 2.15D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1276.01578922796 IErMin= 2 ErrMin= 1.35D-04

ErrMax= 2.15D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.74D-05 BMatP= 1.04D-05

IDIUse=3 WtCom= 4.06D-01 WtEn= 5.94D-01

Coeff-Com: -0.207D-01 0.633D+00 0.387D+00

Coeff-En: 0.000D+00 0.615D+00 0.385D+00

Coeff: -0.838D-02 0.622D+00 0.386D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=4.42D-06 MaxDP=1.84D-04 DE= 2.21D-06 OVMax= 7.63D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 3.09D-06 CP: 1.00D+00 1.16D+00 6.33D-01

E= -1276.01579329141 Delta-E= -0.000006275645 Rises=F Damp=F

DIIS: error= 4.72D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1276.01579329141 IErMin= 4 ErrMin= 4.72D-05

ErrMax= 4.72D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.33D-07 BMatP= 1.04D-05

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

Coeff-Com: -0.108D-01 0.179D+00 0.111D+00 0.721D+00

Coeff: -0.108D-01 0.179D+00 0.111D+00 0.721D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=2.21D-06 MaxDP=1.15D-04 DE=-6.28D-06 OVMax= 1.70D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 9.03D-07 CP: 1.00D+00 1.21D+00 8.42D-01 1.34D+00

E= -1276.01579381953 Delta-E= -0.000000528119 Rises=F Damp=F

DIIS: error= 3.71D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1276.01579381953 IErMin= 5 ErrMin= 3.71D-05

ErrMax= 3.71D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.12D-07 BMatP= 3.33D-07

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

Coeff-Com: -0.106D-03-0.108D-01-0.514D-01 0.364D+00 0.698D+00

Coeff: -0.106D-03-0.108D-01-0.514D-01 0.364D+00 0.698D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=2.03D-06 MaxDP=9.68D-05 DE=-5.28D-07 OVMax= 1.57D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 4.33D-07 CP: 1.00D+00 1.26D+00 9.86D-01 1.80D+00 1.30D+00

E= -1276.01579427590 Delta-E= -0.000000456372 Rises=F Damp=F

DIIS: error= 2.89D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1276.01579427590 IErMin= 6 ErrMin= 2.89D-05

ErrMax= 2.89D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.92D-07 BMatP= 3.12D-07

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

Coeff-Com: 0.101D-01-0.140D+00-0.187D+00-0.574D+00 0.215D+00 0.168D+01

Coeff: 0.101D-01-0.140D+00-0.187D+00-0.574D+00 0.215D+00 0.168D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=5.07D-06 MaxDP=2.50D-04 DE=-4.56D-07 OVMax= 3.97D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 4.10D-07 CP: 1.00D+00 1.39D+00 1.37D+00 2.90D+00 2.67D+00

CP: 2.44D+00

E= -1276.01579503182 Delta-E= -0.000000755922 Rises=F Damp=F

DIIS: error= 1.41D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1276.01579503182 IErMin= 7 ErrMin= 1.41D-05

ErrMax= 1.41D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.22D-08 BMatP= 1.92D-07

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

Coeff-Com: 0.777D-02-0.890D-01-0.121D+00-0.644D+00-0.248D+00 0.121D+01

Coeff-Com: 0.880D+00

Coeff: 0.777D-02-0.890D-01-0.121D+00-0.644D+00-0.248D+00 0.121D+01

Coeff: 0.880D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=3.82D-06 MaxDP=1.89D-04 DE=-7.56D-07 OVMax= 2.97D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.38D-06 CP: 1.00D+00 1.48D+00 1.66D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.39D+00

E= -1276.01579525991 Delta-E= -0.000000228094 Rises=F Damp=F

DIIS: error= 3.99D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1276.01579525991 IErMin= 8 ErrMin= 3.99D-06

ErrMax= 3.99D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.84D-08 BMatP= 7.22D-08

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

Coeff-Com: -0.792D-03 0.306D-01 0.271D-01-0.341D-01-0.209D+00-0.103D+00

Coeff-Com: 0.491D+00 0.798D+00

Coeff: -0.792D-03 0.306D-01 0.271D-01-0.341D-01-0.209D+00-0.103D+00

Coeff: 0.491D+00 0.798D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=7.42D-07 MaxDP=3.97D-05 DE=-2.28D-07 OVMax= 5.55D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.86D-07 CP: 1.00D+00 1.50D+00 1.72D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.70D+00 1.22D+00

E= -1276.01579527394 Delta-E= -0.000000014029 Rises=F Damp=F

DIIS: error= 1.96D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1276.01579527394 IErMin= 9 ErrMin= 1.96D-06

ErrMax= 1.96D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.95D-09 BMatP= 1.84D-08

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

Coeff-Com: -0.177D-02 0.312D-01 0.377D-01 0.876D-01-0.744D-01-0.248D+00

Coeff-Com: 0.107D+00 0.411D+00 0.650D+00

Coeff: -0.177D-02 0.312D-01 0.377D-01 0.876D-01-0.744D-01-0.248D+00

Coeff: 0.107D+00 0.411D+00 0.650D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.18D-07 MaxDP=7.99D-06 DE=-1.40D-08 OVMax= 5.47D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 8.23D-08 CP: 1.00D+00 1.50D+00 1.72D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.78D+00 1.24D+00 1.10D+00

E= -1276.01579527632 Delta-E= -0.000000002375 Rises=F Damp=F

DIIS: error= 1.24D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1276.01579527632 IErMin=10 ErrMin= 1.24D-06

ErrMax= 1.24D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.44D-09 BMatP= 4.95D-09

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

Coeff-Com: -0.637D-03 0.649D-02 0.122D-01 0.572D-01 0.275D-01-0.883D-01

Coeff-Com: -0.881D-01-0.366D-01 0.336D+00 0.774D+00

Coeff: -0.637D-03 0.649D-02 0.122D-01 0.572D-01 0.275D-01-0.883D-01

Coeff: -0.881D-01-0.366D-01 0.336D+00 0.774D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.45D-07 MaxDP=6.16D-06 DE=-2.37D-09 OVMax= 1.04D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 4.81D-08 CP: 1.00D+00 1.50D+00 1.71D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.82D+00 1.20D+00 1.23D+00 1.32D+00

E= -1276.01579527730 Delta-E= -0.000000000986 Rises=F Damp=F

DIIS: error= 5.63D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1276.01579527730 IErMin=11 ErrMin= 5.63D-07

ErrMax= 5.63D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.48D-10 BMatP= 1.44D-09

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

Coeff-Com: 0.236D-03-0.745D-02-0.689D-02 0.277D-02 0.438D-01 0.373D-01

Coeff-Com: -0.875D-01-0.165D+00-0.454D-01 0.407D+00 0.821D+00

Coeff: 0.236D-03-0.745D-02-0.689D-02 0.277D-02 0.438D-01 0.373D-01

Coeff: -0.875D-01-0.165D+00-0.454D-01 0.407D+00 0.821D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=7.88D-08 MaxDP=3.26D-06 DE=-9.86D-10 OVMax= 5.35D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 2.65D-08 CP: 1.00D+00 1.49D+00 1.71D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.83D+00 1.18D+00 1.30D+00 1.64D+00

CP: 1.31D+00

E= -1276.01579527749 Delta-E= -0.000000000185 Rises=F Damp=F

DIIS: error= 3.99D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1276.01579527749 IErMin=12 ErrMin= 3.99D-07

ErrMax= 3.99D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.24D-10 BMatP= 3.48D-10

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

Coeff-Com: 0.237D-03-0.448D-02-0.620D-02-0.116D-01 0.107D-01 0.303D-01

Coeff-Com: -0.162D-01-0.536D-01-0.986D-01 0.159D-01 0.352D+00 0.782D+00

Coeff: 0.237D-03-0.448D-02-0.620D-02-0.116D-01 0.107D-01 0.303D-01

Coeff: -0.162D-01-0.536D-01-0.986D-01 0.159D-01 0.352D+00 0.782D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=5.98D-08 MaxDP=2.82D-06 DE=-1.85D-10 OVMax= 4.43D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.07D-08 CP: 1.00D+00 1.50D+00 1.71D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.84D+00 1.20D+00 1.35D+00 1.73D+00

CP: 1.47D+00 1.09D+00

E= -1276.01579527768 Delta-E= -0.000000000190 Rises=F Damp=F

DIIS: error= 2.05D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1276.01579527768 IErMin=13 ErrMin= 2.05D-07

ErrMax= 2.05D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.54D-11 BMatP= 1.24D-10

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

Coeff-Com: 0.725D-04-0.311D-03-0.190D-02-0.603D-02-0.463D-02 0.378D-02

Coeff-Com: 0.130D-01 0.171D-01-0.536D-01-0.107D+00-0.268D-01 0.433D+00

Coeff-Com: 0.733D+00

Coeff: 0.725D-04-0.311D-03-0.190D-02-0.603D-02-0.463D-02 0.378D-02

Coeff: 0.130D-01 0.171D-01-0.536D-01-0.107D+00-0.268D-01 0.433D+00

Coeff: 0.733D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=3.12D-08 MaxDP=1.38D-06 DE=-1.90D-10 OVMax= 2.31D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 5.96D-09 CP: 1.00D+00 1.50D+00 1.72D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.85D+00 1.21D+00 1.37D+00 1.78D+00

CP: 1.54D+00 1.24D+00 1.25D+00

E= -1276.01579527771 Delta-E= -0.000000000032 Rises=F Damp=F

DIIS: error= 8.72D-08 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1276.01579527771 IErMin=14 ErrMin= 8.72D-08

ErrMax= 8.72D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.00D-12 BMatP= 3.54D-11

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

Coeff-Com: -0.742D-06 0.671D-03 0.178D-04-0.155D-02-0.478D-02-0.439D-02

Coeff-Com: 0.105D-01 0.222D-01-0.129D-01-0.645D-01-0.794D-01 0.819D-01

Coeff-Com: 0.426D+00 0.626D+00

Coeff: -0.742D-06 0.671D-03 0.178D-04-0.155D-02-0.478D-02-0.439D-02

Coeff: 0.105D-01 0.222D-01-0.129D-01-0.645D-01-0.794D-01 0.819D-01

Coeff: 0.426D+00 0.626D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=2.02D-08 MaxDP=9.70D-07 DE=-3.23D-11 OVMax= 1.57D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 2.24D-09 CP: 1.00D+00 1.50D+00 1.72D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.85D+00 1.21D+00 1.38D+00 1.79D+00

CP: 1.55D+00 1.27D+00 1.43D+00 9.93D-01

E= -1276.01579527773 Delta-E= -0.000000000015 Rises=F Damp=F

DIIS: error= 2.90D-08 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1276.01579527773 IErMin=15 ErrMin= 2.90D-08

ErrMax= 2.90D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.10D-12 BMatP= 8.00D-12

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

Coeff-Com: -0.142D-04 0.451D-03 0.387D-03 0.155D-03-0.194D-02-0.350D-02

Coeff-Com: 0.347D-02 0.102D-01 0.308D-02-0.173D-01-0.386D-01-0.403D-01

Coeff-Com: 0.983D-01 0.348D+00 0.638D+00

Coeff: -0.142D-04 0.451D-03 0.387D-03 0.155D-03-0.194D-02-0.350D-02

Coeff: 0.347D-02 0.102D-01 0.308D-02-0.173D-01-0.386D-01-0.403D-01

Coeff: 0.983D-01 0.348D+00 0.638D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=9.19D-09 MaxDP=4.41D-07 DE=-1.55D-11 OVMax= 7.19D-06

Error on total polarization charges = 0.06995

SCF Done: E(UB3LYP) = -1276.01579528 A.U. after 15 cycles

NFock= 15 Conv=0.92D-08 -V/T= 1.9659

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7652 S= 0.5076

<L.S>= 0.000000000000E+00

KE= 1.321004846824D+03 PE=-8.599756956326D+03 EE= 3.242679264886D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.68

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7652, after 0.7501

Leave Link 502 at Tue Sep 17 14:05:17 2019, MaxMem= 2415919104 cpu: 1465.3

(Enter /home/blab/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15317 LenP2D= 41234.

LDataN: DoStor=T MaxTD1= 6 Len= 172

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

GePol: Maximum number of non-zero 1st derivatives = 253

Leave Link 701 at Tue Sep 17 14:05:21 2019, MaxMem= 2415919104 cpu: 71.1

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 14:05:21 2019, MaxMem= 2415919104 cpu: 0.3

(Enter /home/blab/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

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

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

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

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

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Tue Sep 17 14:05:33 2019, MaxMem= 2415919104 cpu: 228.5

(Enter /home/blab/g09/l716.exe)

Dipole = 3.21520588D-13 4.97379915D-14-2.22044605D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000178397 -0.000139663 -0.000000000

2 7 -0.000204609 0.000624733 -0.000000000

3 6 0.000335458 -0.000002892 0.000000000

4 6 -0.000218069 -0.000168393 -0.000000000

5 6 0.000144889 -0.000145765 -0.000000000

6 7 -0.000327413 -0.000095022 -0.000000000

7 6 0.000403425 -0.000056754 0.000000000

8 7 -0.000519696 0.000382753 0.000000000

9 6 0.000366984 -0.000427742 -0.000000000

10 6 -0.000158456 0.000449494 0.000000000

11 6 -0.000230182 -0.000347086 -0.000000000

12 7 0.000164318 -0.000293742 -0.000000000

13 6 0.000158456 -0.000449494 0.000000000

14 6 0.000230182 0.000347086 0.000000000

15 6 -0.000403425 0.000056754 -0.000000000

16 7 0.000519696 -0.000382753 -0.000000000

17 6 -0.000366984 0.000427742 0.000000000

18 7 0.000327413 0.000095022 0.000000000

19 7 0.000204609 -0.000624733 0.000000000

20 6 -0.000335458 0.000002892 -0.000000000

21 6 0.000218069 0.000168393 -0.000000000

22 6 -0.000144889 0.000145765 -0.000000000

23 6 0.000178397 0.000139663 0.000000000

24 7 -0.000164318 0.000293742 -0.000000000

25 30 -0.000000000 0.000000000 0.000000000

26 6 -0.000059092 0.000138629 0.000000000

27 1 0.000004736 -0.000036859 0.000000000

28 6 -0.000072329 -0.000129418 0.000000000

29 1 0.000054679 0.000054136 0.000000000

30 6 0.000072329 0.000129418 -0.000000000

31 1 -0.000054679 -0.000054136 0.000000000

32 6 0.000059092 -0.000138629 -0.000000000

33 1 -0.000004736 0.000036859 0.000000000

34 1 0.000016096 -0.000038397 0.000000000

35 1 0.000026347 -0.000001840 0.000019651

36 1 0.000026347 -0.000001840 -0.000019651

37 1 0.000028516 0.000045844 0.000021686

38 1 0.000028516 0.000045844 -0.000021686

39 1 0.000008917 0.000014819 -0.000000000

40 1 -0.000028516 -0.000045844 0.000021686

41 1 -0.000028516 -0.000045844 -0.000021686

42 1 -0.000008917 -0.000014819 -0.000000000

43 1 -0.000026347 0.000001840 0.000019651

44 1 -0.000026347 0.000001840 -0.000019651

45 1 -0.000016096 0.000038397 0.000000000

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

Cartesian Forces: Max 0.000624733 RMS 0.000184891

Leave Link 716 at Tue Sep 17 14:05:33 2019, MaxMem= 2415919104 cpu: 0.3

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

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

Internal Forces: Max 0.000303318 RMS 0.000079780

Search for a local minimum.

Step number 9 out of a maximum of 270

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

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4 5

6 7 8 9

DE= -2.22D-05 DEPred=-2.21D-05 R= 1.00D+00

TightC=F SS= 1.41D+00 RLast= 1.48D-02 DXNew= 2.9025D-01 4.4464D-02

Trust test= 1.00D+00 RLast= 1.48D-02 DXMaxT set to 1.73D-01

ITU= 1 -1 1 1 1 0 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01329

Eigenvalues --- 0.01330 0.01341 0.01342 0.01608 0.01628

Eigenvalues --- 0.01636 0.01646 0.01771 0.01790 0.01804

Eigenvalues --- 0.01818 0.01886 0.01906 0.01938 0.01948

Eigenvalues --- 0.01997 0.02000 0.02045 0.02048 0.02070

Eigenvalues --- 0.02087 0.02102 0.02110 0.02114 0.02205

Eigenvalues --- 0.02313 0.02317 0.02352 0.02373 0.07115

Eigenvalues --- 0.07183 0.07183 0.07184 0.07184 0.07200

Eigenvalues --- 0.07267 0.07323 0.11477 0.13923 0.14495

Eigenvalues --- 0.14497 0.15119 0.15945 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16001 0.16021

Eigenvalues --- 0.16030 0.16450 0.17980 0.19803 0.22073

Eigenvalues --- 0.22096 0.23375 0.23845 0.23861 0.24316

Eigenvalues --- 0.24398 0.24969 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25060 0.25239

Eigenvalues --- 0.25588 0.27074 0.30042 0.33209 0.33209

Eigenvalues --- 0.33266 0.33282 0.33282 0.33324 0.33560

Eigenvalues --- 0.33723 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33724 0.33856 0.34425 0.34437

Eigenvalues --- 0.34437 0.34439 0.34635 0.35537 0.35548

Eigenvalues --- 0.35682 0.35682 0.35694 0.35749 0.37572

Eigenvalues --- 0.38556 0.41595 0.41774 0.41853 0.43922

Eigenvalues --- 0.47953 0.48966 0.48981 0.51351 0.51361

Eigenvalues --- 0.51363 0.52007 0.53631 0.53758 0.54016

Eigenvalues --- 0.54024 0.56329 0.56334 0.56825

DIIS coeff's: 1.37833 -0.47931 0.06149 -0.02749 0.10272

DIIS coeff's: -0.03575

Cosine: 0.916 > 0.500

Length: 1.215

GDIIS step was calculated using 6 of the last 6 vectors.

Iteration 1 RMS(Cart)= 0.00092510 RMS(Int)= 0.00000082

Iteration 2 RMS(Cart)= 0.00000071 RMS(Int)= 0.00000070

ITry= 1 IFail=0 DXMaxC= 3.86D-03 DCOld= 1.00D+10 DXMaxT= 1.73D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 4.21D-11 for atom 36.

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

(Linear) (Quad) (Total)

R1 2.58236 0.00009 0.00030 0.00027 0.00057 2.58293

R2 2.71223 0.00014 0.00079 -0.00011 0.00068 2.71292

R3 2.58352 -0.00016 -0.00141 0.00023 -0.00118 2.58235

R4 2.58287 0.00017 -0.00026 0.00031 0.00005 2.58292

R5 3.80438 -0.00010 -0.00058 0.00016 -0.00041 3.80397

R6 2.72750 0.00012 0.00093 0.00017 0.00110 2.72860

R7 2.57981 -0.00019 -0.00118 0.00022 -0.00097 2.57884

R8 2.62462 -0.00017 -0.00105 0.00015 -0.00090 2.62371

R9 2.82535 -0.00010 -0.00009 -0.00030 -0.00039 2.82496

R10 2.04551 0.00002 -0.00004 0.00010 0.00006 2.04558

R11 2.50030 0.00013 0.00110 -0.00000 0.00110 2.50140

R12 2.58804 0.00019 -0.00036 0.00054 0.00018 2.58822

R13 2.77837 -0.00014 -0.00080 -0.00011 -0.00091 2.77746

R14 2.58440 0.00015 0.00032 0.00039 0.00071 2.58511

R15 3.79402 -0.00027 -0.00094 -0.00037 -0.00131 3.79271

R16 2.80420 -0.00026 -0.00172 -0.00007 -0.00178 2.80242

R17 2.49634 0.00026 0.00086 0.00003 0.00089 2.49724

R18 2.56716 0.00024 0.00082 0.00014 0.00097 2.56813

R19 2.81614 -0.00002 0.00004 -0.00007 -0.00003 2.81610

R20 2.04516 -0.00002 0.00001 -0.00009 -0.00008 2.04509

R21 2.49634 0.00026 0.00086 0.00003 0.00089 2.49724

R22 2.56716 0.00024 0.00082 0.00014 0.00097 2.56813

R23 2.80420 -0.00026 -0.00172 -0.00007 -0.00178 2.80242

R24 2.81614 -0.00002 0.00004 -0.00007 -0.00003 2.81610

R25 2.77837 -0.00014 -0.00080 -0.00011 -0.00091 2.77746

R26 2.04516 -0.00002 0.00001 -0.00009 -0.00008 2.04509

R27 2.58804 0.00019 -0.00036 0.00054 0.00018 2.58822

R28 2.50030 0.00013 0.00110 -0.00000 0.00110 2.50140

R29 2.58440 0.00015 0.00032 0.00039 0.00071 2.58511

R30 3.79402 -0.00027 -0.00094 -0.00037 -0.00131 3.79271

R31 2.57981 -0.00019 -0.00118 0.00022 -0.00097 2.57884

R32 2.58287 0.00017 -0.00026 0.00031 0.00005 2.58292

R33 2.58236 0.00009 0.00030 0.00027 0.00057 2.58293

R34 3.80438 -0.00010 -0.00058 0.00016 -0.00041 3.80397

R35 2.72750 0.00012 0.00093 0.00017 0.00110 2.72860

R36 2.62462 -0.00017 -0.00105 0.00015 -0.00090 2.62371

R37 2.82535 -0.00010 -0.00009 -0.00030 -0.00039 2.82496

R38 2.71223 0.00014 0.00079 -0.00011 0.00068 2.71292

R39 2.04551 0.00002 -0.00004 0.00010 0.00006 2.04558

R40 2.58352 -0.00016 -0.00141 0.00023 -0.00118 2.58235

R41 2.06451 0.00001 0.00001 0.00002 0.00003 2.06454

R42 2.07009 0.00003 0.00000 0.00007 0.00007 2.07016

R43 2.07009 0.00003 0.00000 0.00007 0.00007 2.07016

R44 2.06888 0.00005 -0.00000 0.00012 0.00012 2.06900

R45 2.06888 0.00005 -0.00000 0.00012 0.00012 2.06900

R46 2.06321 -0.00000 -0.00000 -0.00002 -0.00002 2.06319

R47 2.06888 0.00005 -0.00000 0.00012 0.00012 2.06900

R48 2.06888 0.00005 -0.00000 0.00012 0.00012 2.06900

R49 2.06321 -0.00000 -0.00000 -0.00002 -0.00002 2.06319

R50 2.07009 0.00003 0.00000 0.00007 0.00007 2.07016

R51 2.07009 0.00003 0.00000 0.00007 0.00007 2.07016

R52 2.06451 0.00001 0.00001 0.00002 0.00003 2.06454

A1 1.88843 0.00009 -0.00024 0.00048 0.00024 1.88867

A2 2.20728 -0.00019 -0.00027 -0.00058 -0.00084 2.20644

A3 2.18747 0.00010 0.00051 0.00009 0.00060 2.18808

A4 1.90584 -0.00017 -0.00000 -0.00036 -0.00037 1.90548

A5 2.19018 0.00030 0.00046 0.00085 0.00132 2.19150

A6 2.18716 -0.00013 -0.00046 -0.00049 -0.00095 2.18621

A7 1.89728 0.00006 0.00002 -0.00003 -0.00000 1.89728

A8 2.21414 0.00006 0.00071 -0.00003 0.00068 2.21482

A9 2.17177 -0.00012 -0.00073 0.00005 -0.00068 2.17108

A10 1.85383 0.00002 -0.00003 0.00025 0.00022 1.85405

A11 2.18823 -0.00009 -0.00071 -0.00020 -0.00091 2.18732

A12 2.24112 0.00007 0.00074 -0.00005 0.00070 2.24182

A13 1.87939 -0.00001 0.00026 -0.00034 -0.00009 1.87930

A14 2.18525 0.00003 -0.00020 0.00028 0.00007 2.18532

A15 2.21855 -0.00003 -0.00005 0.00007 0.00001 2.21856

A16 2.17716 0.00005 -0.00026 0.00036 0.00010 2.17726

A17 2.22946 -0.00009 -0.00045 -0.00007 -0.00052 2.22894

A18 2.17454 0.00004 -0.00003 0.00012 0.00009 2.17462

A19 1.87919 0.00005 0.00048 -0.00005 0.00043 1.87962

A20 1.91378 -0.00009 -0.00055 -0.00009 -0.00064 1.91314

A21 2.18888 -0.00003 0.00025 -0.00037 -0.00011 2.18877

A22 2.18052 0.00012 0.00030 0.00046 0.00076 2.18128

A23 1.88598 0.00004 0.00042 -0.00006 0.00037 1.88634

A24 2.23914 -0.00004 -0.00042 0.00004 -0.00038 2.23876

A25 2.15807 0.00000 -0.00000 0.00001 0.00001 2.15809

A26 1.85854 0.00006 0.00006 0.00012 0.00019 1.85872

A27 2.16488 0.00002 0.00029 0.00017 0.00046 2.16534

A28 2.25977 -0.00008 -0.00035 -0.00029 -0.00064 2.25912

A29 1.88729 -0.00006 -0.00042 0.00008 -0.00034 1.88695

A30 2.16909 0.00010 0.00067 0.00021 0.00088 2.16997

A31 2.22680 -0.00004 -0.00025 -0.00029 -0.00054 2.22626

A32 2.17723 -0.00005 0.00013 -0.00019 -0.00006 2.17717

A33 1.85854 0.00006 0.00006 0.00012 0.00019 1.85872

A34 2.25977 -0.00008 -0.00035 -0.00029 -0.00064 2.25912

A35 2.16488 0.00002 0.00029 0.00017 0.00046 2.16534

A36 1.88729 -0.00006 -0.00042 0.00008 -0.00034 1.88695

A37 2.22680 -0.00004 -0.00025 -0.00029 -0.00054 2.22626

A38 2.16909 0.00010 0.00067 0.00021 0.00088 2.16997

A39 1.87919 0.00005 0.00048 -0.00005 0.00043 1.87962

A40 2.17454 0.00004 -0.00003 0.00012 0.00009 2.17462

A41 2.22946 -0.00009 -0.00045 -0.00007 -0.00052 2.22894

A42 1.91378 -0.00009 -0.00055 -0.00009 -0.00064 1.91314

A43 2.18888 -0.00003 0.00025 -0.00037 -0.00011 2.18877

A44 2.18052 0.00012 0.00030 0.00046 0.00076 2.18128

A45 2.15807 0.00000 -0.00000 0.00001 0.00001 2.15809

A46 2.23914 -0.00004 -0.00042 0.00004 -0.00038 2.23876

A47 1.88598 0.00004 0.00042 -0.00006 0.00037 1.88634

A48 2.17716 0.00005 -0.00026 0.00036 0.00010 2.17726

A49 1.90584 -0.00017 -0.00000 -0.00036 -0.00037 1.90548

A50 2.18716 -0.00013 -0.00046 -0.00049 -0.00095 2.18621

A51 2.19018 0.00030 0.00046 0.00085 0.00132 2.19150

A52 2.21414 0.00006 0.00071 -0.00003 0.00068 2.21482

A53 2.17177 -0.00012 -0.00073 0.00005 -0.00068 2.17108

A54 1.89728 0.00006 0.00002 -0.00003 -0.00000 1.89728

A55 1.85383 0.00002 -0.00003 0.00025 0.00022 1.85405

A56 2.18823 -0.00009 -0.00071 -0.00020 -0.00091 2.18732

A57 2.24112 0.00007 0.00074 -0.00005 0.00070 2.24182

A58 1.87939 -0.00001 0.00026 -0.00034 -0.00009 1.87930

A59 2.21855 -0.00003 -0.00005 0.00007 0.00001 2.21856

A60 2.18525 0.00003 -0.00020 0.00028 0.00007 2.18532

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A62 2.20728 -0.00019 -0.00027 -0.00058 -0.00084 2.20644

A63 2.18747 0.00010 0.00051 0.00009 0.00060 2.18808

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A65 1.56957 0.00014 0.00021 0.00059 0.00080 1.57037

A66 1.57202 -0.00014 -0.00021 -0.00059 -0.00080 1.57122

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A69 1.94141 0.00006 0.00053 0.00006 0.00059 1.94200

A70 1.94979 -0.00002 -0.00013 -0.00006 -0.00018 1.94961

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A72 1.88072 -0.00001 0.00000 -0.00000 -0.00000 1.88072

A73 1.88072 -0.00001 0.00000 -0.00000 -0.00000 1.88072

A74 1.85729 -0.00000 -0.00031 0.00007 -0.00025 1.85705

A75 1.93953 0.00002 0.00011 0.00012 0.00024 1.93977

A76 1.93953 0.00002 0.00011 0.00012 0.00024 1.93977

A77 1.94547 0.00001 0.00025 -0.00014 0.00011 1.94558

A78 1.85777 -0.00004 -0.00025 -0.00011 -0.00036 1.85741

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A80 1.88915 -0.00001 -0.00013 0.00000 -0.00013 1.88902

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A83 1.94547 0.00001 0.00025 -0.00014 0.00011 1.94558

A84 1.85777 -0.00004 -0.00025 -0.00011 -0.00036 1.85741

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A90 1.85729 -0.00000 -0.00031 0.00007 -0.00025 1.85705

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A96 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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D15 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

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D17 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D18 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D19 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D20 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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D23 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

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D31 -1.03916 0.00001 0.00028 -0.00001 0.00028 -1.03888

D32 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.10243 -0.00001 -0.00028 0.00001 -0.00028 -2.10271

D34 2.10243 0.00001 0.00028 -0.00001 0.00028 2.10271

D35 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

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D56 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D57 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D58 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D59 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D60 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D61 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D62 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D63 1.03267 -0.00001 -0.00008 0.00001 -0.00007 1.03260

D64 -1.03267 0.00001 0.00008 -0.00001 0.00007 -1.03260

D65 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D66 -2.10893 -0.00001 -0.00008 0.00001 -0.00007 -2.10900

D67 2.10893 0.00001 0.00008 -0.00001 0.00007 2.10900

D68 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D69 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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D76 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D77 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D78 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D79 -2.10893 -0.00001 -0.00008 0.00001 -0.00007 -2.10900

D80 2.10893 0.00001 0.00008 -0.00001 0.00007 2.10900

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 1.03267 -0.00001 -0.00008 0.00001 -0.00007 1.03260

D83 -1.03267 0.00001 0.00008 -0.00001 0.00007 -1.03260

D84 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D85 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D86 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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D104 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D105 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D106 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D107 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D108 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D109 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

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D111 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D112 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D113 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D114 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D115 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D116 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D117 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D118 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D119 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D120 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

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D122 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D123 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D124 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D125 1.03916 -0.00001 -0.00028 0.00001 -0.00028 1.03888

D126 -1.03916 0.00001 0.00028 -0.00001 0.00028 -1.03888

D127 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D128 -2.10243 -0.00001 -0.00028 0.00001 -0.00028 -2.10271

D129 2.10243 0.00001 0.00028 -0.00001 0.00028 2.10271

D130 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D131 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D132 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D133 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D134 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D135 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D136 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

Item Value Threshold Converged?

Maximum Force 0.000303 0.000450 YES

RMS Force 0.000080 0.000300 YES

Maximum Displacement 0.003856 0.001800 NO

RMS Displacement 0.000925 0.001200 YES

Predicted change in Energy=-3.020927D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:05:33 2019, MaxMem= 2415919104 cpu: 1.1

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.074734 -2.194584 -0.000000

2 7 0 -0.747215 -1.869152 -0.000000

3 6 0 -0.003797 -3.016115 -0.000000

4 6 0 -0.899574 -4.148575 -0.000000

5 6 0 -2.185841 -3.625893 -0.000000

6 7 0 1.357624 -3.110126 -0.000000

7 6 0 2.185207 -2.077052 -0.000000

8 7 0 1.863307 -0.745791 -0.000000

9 6 0 3.007882 0.003424 -0.000000

10 6 0 4.165038 -0.924051 -0.000000

11 6 0 3.651214 -2.182164 -0.000000

12 7 0 -3.124514 -1.319748 -0.000000

13 6 0 -4.165038 0.924051 -0.000000

14 6 0 -3.651214 2.182164 -0.000000

15 6 0 -2.185207 2.077052 -0.000000

16 7 0 -1.863307 0.745791 -0.000000

17 6 0 -3.007882 -0.003424 -0.000000

18 7 0 -1.357624 3.110126 -0.000000

19 7 0 0.747215 1.869152 -0.000000

20 6 0 0.003797 3.016115 -0.000000

21 6 0 0.899574 4.148575 -0.000000

22 6 0 2.185841 3.625893 -0.000000

23 6 0 2.074734 2.194584 -0.000000

24 7 0 3.124514 1.319748 -0.000000

25 30 0 0.000000 -0.000000 -0.000000

26 6 0 -0.479202 -5.583158 -0.000000

27 1 0 -3.115923 -4.179695 -0.000000

28 6 0 5.588435 -0.482816 -0.000000

29 1 0 4.196060 -3.117219 -0.000000

30 6 0 -5.588435 0.482816 -0.000000

31 1 0 -4.196060 3.117219 -0.000000

32 6 0 0.479202 5.583158 -0.000000

33 1 0 3.115923 4.179695 -0.000000

34 1 0 -1.344778 -6.249754 -0.000000

35 1 0 0.130113 -5.826778 0.877194

36 1 0 0.130113 -5.826778 -0.877194

37 1 0 5.810612 0.134079 0.876821

38 1 0 5.810612 0.134079 -0.876821

39 1 0 6.271017 -1.334930 -0.000000

40 1 0 -5.810612 -0.134079 0.876821

41 1 0 -5.810612 -0.134079 -0.876821

42 1 0 -6.271017 1.334930 -0.000000

43 1 0 -0.130113 5.826778 0.877194

44 1 0 -0.130113 5.826778 -0.877194

45 1 0 1.344778 6.249754 -0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.366826 0.000000

3 C 2.227935 1.366820 0.000000

4 C 2.280150 2.284510 1.443912 0.000000

5 C 1.435614 2.270635 2.265644 1.388409 0.000000

6 N 3.552365 2.443433 1.364663 2.484616 3.580804

7 C 4.261563 2.939783 2.381928 3.715788 4.637345

8 N 4.196090 2.841965 2.939464 4.383201 4.968962

9 C 5.537530 4.196105 4.264720 5.701519 6.336142

10 C 6.367811 5.002345 4.664325 6.003987 6.901711

11 C 5.725962 4.409553 3.748944 4.957463 6.012949

12 N 1.366519 2.439957 3.551976 3.598975 2.489861

13 C 3.754365 4.414011 5.730693 6.032810 4.961775

14 C 4.652012 4.984613 6.350257 6.902882 5.990062

15 C 4.273064 4.200041 5.540659 6.356987 5.702945

16 N 2.947967 2.843164 4.196393 4.988347 4.383565

17 C 2.381585 2.931135 4.254508 4.650510 3.714570

18 N 5.352962 5.016553 6.274048 7.273139 6.786744

19 N 4.947459 4.025945 4.942657 6.238986 6.228831

20 C 5.609963 4.942657 6.032236 7.221418 6.993625

21 C 7.005868 6.238986 7.221418 8.489973 8.364337

22 C 7.213214 6.228831 6.993625 8.364337 8.467585

23 C 6.040107 4.947459 5.609963 7.005868 7.213214

24 N 6.275565 5.015912 5.346592 6.789392 7.256668

25 Zn 3.020053 2.012973 3.016118 4.244986 4.233792

26 C 3.745418 3.723664 2.610693 1.494905 2.596826

27 H 2.241593 3.308986 3.322536 2.216568 1.082474

28 C 7.852026 6.485553 6.139272 7.451983 8.385600

29 H 6.338305 5.098396 4.201074 5.198959 6.402141

30 C 4.417529 5.382300 6.590197 6.590539 5.334710

31 H 5.719727 6.062872 7.429190 7.978633 7.036372

32 C 8.186322 7.552550 8.612827 9.828919 9.586921

33 H 8.220363 7.177213 7.842980 9.245772 9.435884

34 H 4.120344 4.421172 3.500664 2.147826 2.755365

35 H 4.338623 4.147527 2.947410 2.155479 3.313157

36 H 4.338623 4.147527 2.947410 2.155479 3.313157

37 H 8.268626 6.912803 6.670824 8.008529 8.879722

38 H 8.268626 6.912803 6.670824 8.008529 8.879722

39 H 8.389909 7.038536 6.496128 7.702855 8.761676

40 H 4.355603 5.423770 6.541716 6.403382 5.108869

41 H 4.355603 5.423770 6.541716 6.403382 5.108869

42 H 5.483271 6.385806 7.629524 7.676017 6.426385

43 H 8.300197 7.770303 8.887192 10.043366 9.713314

44 H 8.300197 7.770303 8.887192 10.043366 9.713314

45 H 9.110429 8.384096 9.363492 10.637780 10.487786

6 7 8 9 10

6 N 0.000000

7 C 1.323683 0.000000

8 N 2.417808 1.369626 0.000000

9 C 3.523854 2.237225 1.367983 0.000000

10 C 3.558160 2.291101 2.308624 1.482977 0.000000

11 C 2.474201 1.469770 2.293421 2.278305 1.358994

12 N 4.826491 5.363455 5.020735 6.273521 7.300284

13 C 6.839180 7.023691 6.255343 7.231760 8.532623

14 C 7.286755 7.225284 6.243625 7.006459 8.410848

15 C 6.281598 6.029685 4.935474 5.591790 7.023691

16 N 5.024191 4.935474 4.014033 4.927432 6.255343

17 C 5.358101 5.591790 4.927432 6.015769 7.231760

18 N 6.787054 6.281598 5.024191 5.358101 6.839180

19 N 5.016553 4.200041 2.843164 2.931135 4.414011

20 C 6.274048 5.540659 4.196393 4.254508 5.730693

21 C 7.273139 6.356987 4.988347 4.650510 6.032810

22 C 6.786744 5.702945 4.383565 3.714570 4.961775

23 C 5.352962 4.273064 2.947967 2.381585 3.754365

24 N 4.769244 3.524280 2.420144 1.321481 2.473323

25 Zn 3.393527 3.014843 2.007017 3.007884 4.266312

26 C 3.080554 4.403618 5.374706 6.585564 6.578468

27 H 4.599631 5.702902 6.048506 7.416164 7.975689

28 C 4.980213 3.758131 3.734399 2.625963 1.490217

29 H 2.838445 2.263951 3.326471 3.339189 2.193387

30 C 7.820292 8.184280 7.552346 8.609674 9.854416

31 H 8.344054 8.228063 7.186012 7.848089 9.286540

32 C 8.737552 7.847883 6.478529 6.125982 7.478580

33 H 7.498874 6.325592 5.082269 4.177668 5.210457

34 H 4.142492 5.465550 6.370668 7.618917 7.662975

35 H 3.107483 4.365012 5.439656 6.560662 6.409901

36 H 3.107483 4.365012 5.439656 6.560662 6.409901

37 H 5.578780 4.336067 4.138140 2.939588 2.143914

38 H 5.578780 4.336067 4.138140 2.939588 2.143914

39 H 5.224247 4.152661 4.446909 3.526931 2.145686

40 H 7.810844 8.275088 7.748034 8.863045 10.045221

41 H 7.810844 8.275088 7.748034 8.863045 10.045221

42 H 8.829195 9.118627 8.396227 9.373947 10.677746

43 H 9.102257 8.282554 6.924005 6.672925 8.049316

44 H 9.102257 8.282554 6.924005 6.672925 8.049316

45 H 9.359889 8.369111 7.014736 6.463942 7.708265

11 12 13 14 15

11 C 0.000000

12 N 6.830391 0.000000

13 C 8.410848 2.473323 0.000000

14 C 8.507221 3.541299 1.358994 0.000000

15 C 7.225284 3.524280 2.291101 1.469770 0.000000

16 N 6.243625 2.420144 2.308624 2.293421 1.369626

17 C 7.006459 1.321481 1.482977 2.278305 2.237225

18 N 7.286755 4.769244 3.558160 2.474201 1.323683

19 N 4.984613 5.015912 5.002345 4.409553 2.939783

20 C 6.350257 5.346592 4.664325 3.748944 2.381928

21 C 6.902882 6.789392 6.003987 4.957463 3.715788

22 C 5.990062 7.256668 6.901711 6.012949 4.637345

23 C 4.652012 6.275565 6.367811 5.725962 4.261563

24 N 3.541299 6.783604 7.300284 6.830391 5.363455

25 Zn 4.253611 3.391802 4.266312 4.253611 3.014843

26 C 5.350429 5.017404 7.478580 8.388199 7.847883

27 H 7.055797 2.859960 5.210457 6.384339 6.325592

28 C 2.576938 8.753053 9.854416 9.616300 8.184280

29 H 1.082213 7.538017 9.286540 9.469064 8.228063

30 C 9.616300 3.052891 1.490217 2.576938 3.758131

31 H 9.469064 4.564525 2.193387 1.082213 2.263951

32 C 8.388199 7.786968 6.578468 5.350429 4.403618

33 H 6.384339 8.317868 7.975689 7.055797 5.702902

34 H 6.442455 5.241414 7.708265 8.741675 8.369111

35 H 5.143037 5.628089 8.049316 8.900059 8.282554

36 H 5.143037 5.628089 8.049316 8.900059 8.282554

37 H 3.285848 9.094993 10.045221 9.720577 8.275088

38 H 3.285848 9.094993 10.045221 9.720577 8.275088

39 H 2.753394 9.395543 10.677746 10.527137 9.118627

40 H 9.720577 3.064270 2.143914 3.285848 4.336067

41 H 9.720577 3.064270 2.143914 3.285848 4.336067

42 H 10.527137 4.116770 2.145686 2.753394 4.152661

43 H 8.900059 7.797996 6.409901 5.143037 4.365012

44 H 8.900059 7.797996 6.409901 5.143037 4.365012

45 H 8.741675 8.790445 7.662975 6.442455 5.465550

16 17 18 19 20

16 N 0.000000

17 C 1.367983 0.000000

18 N 2.417808 3.523854 0.000000

19 N 2.841965 4.196105 2.443433 0.000000

20 C 2.939464 4.264720 1.364663 1.366820 0.000000

21 C 4.383201 5.701519 2.484616 2.284510 1.443912

22 C 4.968962 6.336142 3.580804 2.270635 2.265644

23 C 4.196090 5.537530 3.552365 1.366826 2.227935

24 N 5.020735 6.273521 4.826491 2.439957 3.551976

25 Zn 2.007017 3.007884 3.393527 2.012973 3.016118

26 C 6.478529 6.125982 8.737552 7.552550 8.612827

27 H 5.082269 4.177668 7.498874 7.177213 7.842980

28 C 7.552346 8.609674 7.820292 5.382300 6.590197

29 H 7.186012 7.848089 8.344054 6.062872 7.429190

30 C 3.734399 2.625963 4.980213 6.485553 6.139272

31 H 3.326471 3.339189 2.838445 5.098396 4.201074

32 C 5.374706 6.585564 3.080554 3.723664 2.610693

33 H 6.048506 7.416164 4.599631 3.308986 3.322536

34 H 7.014736 6.463942 9.359889 8.384096 9.363492

35 H 6.924005 6.672925 9.102257 7.770303 8.887192

36 H 6.924005 6.672925 9.102257 7.770303 8.887192

37 H 7.748034 8.863045 7.810844 5.423770 6.541716

38 H 7.748034 8.863045 7.810844 5.423770 6.541716

39 H 8.396227 9.373947 8.829195 6.385806 7.629524

40 H 4.138140 2.939588 5.578780 6.912803 6.670824

41 H 4.138140 2.939588 5.578780 6.912803 6.670824

42 H 4.446909 3.526931 5.224247 7.038536 6.496128

43 H 5.439656 6.560662 3.107483 4.147527 2.947410

44 H 5.439656 6.560662 3.107483 4.147527 2.947410

45 H 6.370668 7.618917 4.142492 4.421172 3.500664

21 22 23 24 25

21 C 0.000000

22 C 1.388409 0.000000

23 C 2.280150 1.435614 0.000000

24 N 3.598975 2.489861 1.366519 0.000000

25 Zn 4.244986 4.233792 3.020053 3.391802 0.000000

26 C 9.828919 9.586921 8.186322 7.786968 5.603685

27 H 9.245772 9.435884 8.220363 8.317868 5.213332

28 C 6.590539 5.334710 4.417529 3.052891 5.609253

29 H 7.978633 7.036372 5.719727 4.564525 5.227234

30 C 7.451983 8.385600 7.852026 8.753053 5.609253

31 H 5.198959 6.402141 6.338305 7.538017 5.227234

32 C 1.494905 2.596826 3.745418 5.017404 5.603685

33 H 2.216568 1.082474 2.241593 2.859960 5.213332

34 H 10.637780 10.487786 9.110429 8.790445 6.392797

35 H 10.043366 9.713314 8.300197 7.797996 5.893873

36 H 10.043366 9.713314 8.300197 7.797996 5.893873

37 H 6.403382 5.108869 4.355603 3.064270 5.877925

38 H 6.403382 5.108869 4.355603 3.064270 5.877925

39 H 7.676017 6.426385 5.483271 4.116770 6.411528

40 H 8.008529 8.879722 8.268626 9.094993 5.877925

41 H 8.008529 8.879722 8.268626 9.094993 5.877925

42 H 7.702855 8.761676 8.389909 9.395543 6.411528

43 H 2.155479 3.313157 4.338623 5.628089 5.893873

44 H 2.155479 3.313157 4.338623 5.628089 5.893873

45 H 2.147826 2.755365 4.120344 5.241414 6.392797

26 27 28 29 30

26 C 0.000000

27 H 2.986973 0.000000

28 C 7.926519 9.456890 0.000000

29 H 5.285729 7.388772 2.979730 0.000000

30 C 7.930971 5.277530 11.218505 10.425766 0.000000

31 H 9.461057 7.376425 10.425766 10.454467 2.979730

32 C 11.207370 10.403760 7.930971 9.461057 7.926519

33 H 10.403760 10.426663 5.277530 7.376425 9.456890

34 H 1.092507 2.724353 9.018149 6.365034 7.958399

35 H 1.095484 3.744209 7.688997 4.964182 8.560504

36 H 1.095484 3.744209 7.688997 4.964182 8.560504

37 H 8.545020 9.952914 1.094869 3.734505 11.438038

38 H 8.545020 9.952914 1.094869 3.734505 11.438038

39 H 7.975770 9.808534 1.091795 2.735325 11.997950

40 H 7.673670 4.939350 11.438038 10.478618 1.094869

41 H 7.673670 4.939350 11.438038 10.478618 1.094869

42 H 9.022475 6.353401 11.997950 11.374591 1.091795

43 H 11.448928 10.479219 8.560504 9.973982 7.688997

44 H 11.448928 10.479219 8.560504 9.973982 7.688997

45 H 11.972665 11.343336 7.958399 9.791322 9.018149

31 32 33 34 35

31 H 0.000000

32 C 5.285729 0.000000

33 H 7.388772 2.986973 0.000000

34 H 9.791322 11.972665 11.343336 0.000000

35 H 9.973982 11.448928 10.479219 1.767394 0.000000

36 H 9.973982 11.448928 10.479219 1.767394 1.754389

37 H 10.478618 7.673670 4.939350 9.629213 8.234068

38 H 10.478618 7.673670 4.939350 9.629213 8.418815

39 H 11.374591 9.022475 6.353401 9.063986 7.658778

40 H 3.734505 8.545020 9.952914 7.623252 8.227942

41 H 3.734505 8.545020 9.952914 7.623252 8.412824

42 H 2.735325 7.975770 9.808534 9.044073 9.645413

43 H 4.964182 1.095484 3.744209 12.169121 11.656461

44 H 4.964182 1.095484 3.744209 12.169121 11.787746

45 H 6.365034 1.092507 2.724353 12.785594 12.169121

36 37 38 39 40

36 H 0.000000

37 H 8.418815 0.000000

38 H 8.234068 1.753643 0.000000

39 H 7.658778 1.771658 1.771658 0.000000

40 H 8.412824 11.624317 11.755850 12.172782 0.000000

41 H 8.227942 11.755850 11.624317 12.172782 1.753643

42 H 9.645413 12.172782 12.172782 12.823057 1.771658

43 H 11.787746 8.227942 8.412824 9.645413 8.234068

44 H 11.656461 8.412824 8.227942 9.645413 8.418815

45 H 12.169121 7.623252 7.623252 9.044073 9.629213

41 42 43 44 45

41 H 0.000000

42 H 1.771658 0.000000

43 H 8.418815 7.658778 0.000000

44 H 8.234068 7.658778 1.754389 0.000000

45 H 9.629213 9.063986 1.767394 1.767394 0.000000

Stoichiometry C20H16N8Zn(1-,2)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=3 Diff= 2.00D-04

Largest Abelian subgroup C2H NOp 4

Largest concise Abelian subgroup C2H NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.948156 0.655057 0.000000

2 7 0 -1.987775 -0.317507 0.000000

3 6 0 -2.590921 -1.544052 0.000000

4 6 0 -4.022548 -1.356103 0.000000

5 6 0 -4.233762 0.016146 0.000000

6 7 0 -1.973189 -2.760897 0.000000

7 6 0 -0.661857 -2.941296 0.000000

8 7 0 0.315731 -1.982027 0.000000

9 6 0 1.546027 -2.580149 0.000000

10 6 0 1.343539 -4.049237 0.000000

11 6 0 0.000000 -4.253611 0.000000

12 7 0 -2.735766 2.004970 0.000000

13 6 0 -1.343539 4.049237 0.000000

14 6 0 0.000000 4.253611 0.000000

15 6 0 0.661857 2.941296 0.000000

16 7 0 -0.315731 1.982027 0.000000

17 6 0 -1.546027 2.580149 0.000000

18 7 0 1.973189 2.760897 0.000000

19 7 0 1.987775 0.317507 0.000000

20 6 0 2.590921 1.544052 0.000000

21 6 0 4.022548 1.356103 0.000000

22 6 0 4.233762 -0.016146 0.000000

23 6 0 2.948156 -0.655057 0.000000

24 7 0 2.735766 -2.004970 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -5.038308 -2.452904 0.000000

27 1 0 -5.186280 0.530402 0.000000

28 6 0 2.452509 -5.044692 0.000000

29 1 0 -0.523118 -5.200992 0.000000

30 6 0 -2.452509 5.044692 0.000000

31 1 0 0.523118 5.200992 0.000000

32 6 0 5.038308 2.452904 0.000000

33 1 0 5.186280 -0.530402 0.000000

34 1 0 -6.054554 -2.051884 0.000000

35 1 0 -4.934839 -3.100908 0.877194

36 1 0 -4.934839 -3.100908 -0.877194

37 1 0 3.096019 -4.918928 0.876821

38 1 0 3.096019 -4.918928 -0.876821

39 1 0 2.071246 -6.067754 0.000000

40 1 0 -3.096019 4.918928 0.876821

41 1 0 -3.096019 4.918928 -0.876821

42 1 0 -2.071246 6.067754 0.000000

43 1 0 4.934839 3.100908 0.877194

44 1 0 4.934839 3.100908 -0.877194

45 1 0 6.054554 2.051884 0.000000

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

Rotational constants (GHZ): 0.1827628 0.1816986 0.0913188

Leave Link 202 at Tue Sep 17 14:05:33 2019, MaxMem= 2415919104 cpu: 0.2

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 229 symmetry adapted cartesian basis functions of AG symmetry.

There are 82 symmetry adapted cartesian basis functions of BG symmetry.

There are 78 symmetry adapted cartesian basis functions of AU symmetry.

There are 218 symmetry adapted cartesian basis functions of BU symmetry.

There are 212 symmetry adapted basis functions of AG symmetry.

There are 82 symmetry adapted basis functions of BG symmetry.

There are 78 symmetry adapted basis functions of AU symmetry.

There are 204 symmetry adapted basis functions of BU symmetry.

576 basis functions, 1015 primitive gaussians, 607 cartesian basis functions

103 alpha electrons 102 beta electrons

nuclear repulsion energy 2760.3076517218 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= 45 NActive= 45 NUniq= 21 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1141583975 Hartrees.

Nuclear repulsion after empirical dispersion term = 2760.1934933242 Hartrees.

No density basis found on file 724.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

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 = 45

GePol: Total number of spheres = 45

GePol: Number of exposed spheres = 45 (100.00%)

GePol: Number of points = 3614

GePol: Average weight of points = 0.10

GePol: Minimum weight of points = 0.63D-10

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 278

GePol: Fraction of low-weight points (<1% of avg) = 7.69%

GePol: Cavity surface area = 378.829 Ang\*\*2

GePol: Cavity volume = 378.215 Ang\*\*3

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

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

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PCM non-electrostatic energy = -0.0106443268 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2760.1828489975 Hartrees.

Leave Link 301 at Tue Sep 17 14:05:34 2019, MaxMem= 2415919104 cpu: 1.7

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15317 LenP2D= 41234.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.79D-04 NBF= 212 82 78 204

NBsUse= 576 1.00D-06 EigRej= -1.00D+00 NBFU= 212 82 78 204

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= 594 594 594 594 594 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Tue Sep 17 14:05:34 2019, MaxMem= 2415919104 cpu: 11.2

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:05:34 2019, MaxMem= 2415919104 cpu: 1.2

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

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

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000000 -0.000000 -0.000044 Ang= -0.01 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

Occupied (BU) (AG) (BU) (AG) (BU) (AG) (BU) (AG) (BU) (AG)

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(AU) (BU) (AG) (AU) (BG) (BG) (AG) (BU) (AG) (BU)

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

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7652 S= 0.5076

Leave Link 401 at Tue Sep 17 14:05:35 2019, MaxMem= 2415919104 cpu: 19.9

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1141655 IEndB= 1141655 NGot= 2415919104 MDV= 2415163146

LenX= 2415163146 LenY= 2414794090

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= 670000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 39182988.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.66D-15 for 3613.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.39D-15 for 3596 3452.

Iteration 1 A^-1\*A deviation from unit magnitude is 8.55D-15 for 3613.

Iteration 1 A^-1\*A deviation from orthogonality is 1.38D-12 for 1757 1747.

E= -1276.01579241269

DIIS: error= 9.86D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1276.01579241269 IErMin= 1 ErrMin= 9.86D-05

ErrMax= 9.86D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.93D-05 BMatP= 1.93D-05

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

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 0.294 Goal= None Shift= 0.000

Gap= 0.343 Goal= None Shift= 0.000

RMSDP=6.85D-06 MaxDP=1.65D-04 OVMax= 1.35D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 6.85D-06 CP: 1.00D+00

E= -1276.01579910576 Delta-E= -0.000006693063 Rises=F Damp=F

DIIS: error= 1.76D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1276.01579910576 IErMin= 2 ErrMin= 1.76D-05

ErrMax= 1.76D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.54D-07 BMatP= 1.93D-05

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

Coeff-Com: 0.205D-01 0.980D+00

Coeff: 0.205D-01 0.980D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.42D-06 MaxDP=6.38D-05 DE=-6.69D-06 OVMax= 2.10D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.42D-06 CP: 1.00D+00 1.01D+00

E= -1276.01579899445 Delta-E= 0.000000111309 Rises=F Damp=F

DIIS: error= 3.47D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1276.01579910576 IErMin= 2 ErrMin= 1.76D-05

ErrMax= 3.47D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.38D-06 BMatP= 8.54D-07

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

Coeff-Com: -0.149D-01 0.577D+00 0.438D+00

Coeff: -0.149D-01 0.577D+00 0.438D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.03D-06 MaxDP=4.85D-05 DE= 1.11D-07 OVMax= 2.25D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 5.91D-07 CP: 1.00D+00 1.05D+00 4.40D-01

E= -1276.01579930752 Delta-E= -0.000000313069 Rises=F Damp=F

DIIS: error= 9.12D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1276.01579930752 IErMin= 4 ErrMin= 9.12D-06

ErrMax= 9.12D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.13D-07 BMatP= 8.54D-07

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

Coeff-Com: -0.988D-02 0.153D+00 0.247D+00 0.610D+00

Coeff: -0.988D-02 0.153D+00 0.247D+00 0.610D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=2.89D-07 MaxDP=1.18D-05 DE=-3.13D-07 OVMax= 1.07D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.16D-07 CP: 1.00D+00 1.05D+00 5.71D-01 9.09D-01

E= -1276.01579933549 Delta-E= -0.000000027968 Rises=F Damp=F

DIIS: error= 3.63D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1276.01579933549 IErMin= 5 ErrMin= 3.63D-06

ErrMax= 3.63D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.57D-09 BMatP= 1.13D-07

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

Coeff-Com: -0.410D-02 0.477D-01 0.113D+00 0.316D+00 0.527D+00

Coeff: -0.410D-02 0.477D-01 0.113D+00 0.316D+00 0.527D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.24D-07 MaxDP=6.28D-06 DE=-2.80D-08 OVMax= 8.46D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 8.99D-08 CP: 1.00D+00 1.05D+00 5.86D-01 1.02D+00 1.20D+00

E= -1276.01579933857 Delta-E= -0.000000003083 Rises=F Damp=F

DIIS: error= 2.56D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1276.01579933857 IErMin= 6 ErrMin= 2.56D-06

ErrMax= 2.56D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.56D-09 BMatP= 7.57D-09

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

Coeff-Com: 0.207D-03-0.107D-01 0.843D-02 0.176D-01 0.235D+00 0.750D+00

Coeff: 0.207D-03-0.107D-01 0.843D-02 0.176D-01 0.235D+00 0.750D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.45D-07 MaxDP=6.76D-06 DE=-3.08D-09 OVMax= 1.10D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 6.09D-08 CP: 1.00D+00 1.06D+00 6.08D-01 1.15D+00 1.61D+00

CP: 1.51D+00

E= -1276.01579934097 Delta-E= -0.000000002398 Rises=F Damp=F

DIIS: error= 2.11D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1276.01579934097 IErMin= 7 ErrMin= 2.11D-06

ErrMax= 2.11D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.34D-10 BMatP= 1.56D-09

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

Coeff-Com: 0.132D-02-0.197D-01-0.266D-01-0.942D-01-0.679D-01 0.296D+00

Coeff-Com: 0.911D+00

Coeff: 0.132D-02-0.197D-01-0.266D-01-0.942D-01-0.679D-01 0.296D+00

Coeff: 0.911D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.66D-07 MaxDP=8.33D-06 DE=-2.40D-09 OVMax= 1.30D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.46D-08 CP: 1.00D+00 1.06D+00 6.30D-01 1.29D+00 2.10D+00

CP: 2.40D+00 1.71D+00

E= -1276.01579934308 Delta-E= -0.000000002115 Rises=F Damp=F

DIIS: error= 1.57D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1276.01579934308 IErMin= 8 ErrMin= 1.57D-06

ErrMax= 1.57D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.59D-10 BMatP= 7.34D-10

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

Coeff-Com: 0.410D-03 0.214D-02-0.151D-01-0.618D-01-0.245D+00-0.541D+00

Coeff-Com: 0.589D+00 0.127D+01

Coeff: 0.410D-03 0.214D-02-0.151D-01-0.618D-01-0.245D+00-0.541D+00

Coeff: 0.589D+00 0.127D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=2.68D-07 MaxDP=1.29D-05 DE=-2.11D-09 OVMax= 2.08D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 7.31D-08 CP: 1.00D+00 1.06D+00 6.63D-01 1.51D+00 2.88D+00

CP: 3.00D+00 3.00D+00 1.76D+00

E= -1276.01579934526 Delta-E= -0.000000002178 Rises=F Damp=F

DIIS: error= 8.21D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1276.01579934526 IErMin= 9 ErrMin= 8.21D-07

ErrMax= 8.21D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.96D-10 BMatP= 4.59D-10

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

Coeff-Com: -0.426D-03 0.126D-01 0.489D-02 0.125D-01-0.116D+00-0.524D+00

Coeff-Com: -0.282D-01 0.869D+00 0.769D+00

Coeff: -0.426D-03 0.126D-01 0.489D-02 0.125D-01-0.116D+00-0.524D+00

Coeff: -0.282D-01 0.869D+00 0.769D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.53D-07 MaxDP=7.88D-06 DE=-2.18D-09 OVMax= 1.20D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 8.29D-08 CP: 1.00D+00 1.06D+00 6.79D-01 1.63D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.58D+00 2.05D+00

E= -1276.01579934586 Delta-E= -0.000000000601 Rises=F Damp=F

DIIS: error= 4.24D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1276.01579934586 IErMin=10 ErrMin= 4.24D-07

ErrMax= 4.24D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.98D-11 BMatP= 1.96D-10

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

Coeff-Com: -0.378D-03 0.692D-02 0.631D-02 0.262D-01 0.420D-02-0.171D+00

Coeff-Com: -0.202D+00 0.120D+00 0.494D+00 0.716D+00

Coeff: -0.378D-03 0.692D-02 0.631D-02 0.262D-01 0.420D-02-0.171D+00

Coeff: -0.202D+00 0.120D+00 0.494D+00 0.716D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=7.67D-08 MaxDP=3.71D-06 DE=-6.01D-10 OVMax= 5.89D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.56D-08 CP: 1.00D+00 1.06D+00 6.86D-01 1.69D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.88D+00 2.62D+00 1.60D+00

E= -1276.01579934597 Delta-E= -0.000000000112 Rises=F Damp=F

DIIS: error= 1.32D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1276.01579934597 IErMin=11 ErrMin= 1.32D-07

ErrMax= 1.32D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.25D-11 BMatP= 7.98D-11

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

Coeff-Com: -0.477D-04-0.845D-03 0.137D-02 0.810D-02 0.397D-01 0.901D-01

Coeff-Com: -0.557D-01-0.215D+00-0.168D-01 0.275D+00 0.875D+00

Coeff: -0.477D-04-0.845D-03 0.137D-02 0.810D-02 0.397D-01 0.901D-01

Coeff: -0.557D-01-0.215D+00-0.168D-01 0.275D+00 0.875D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.45D-08 MaxDP=8.40D-07 DE=-1.12D-10 OVMax= 1.04D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 5.76D-09 CP: 1.00D+00 1.06D+00 6.87D-01 1.70D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.72D+00 1.70D+00

CP: 1.08D+00

E= -1276.01579934600 Delta-E= -0.000000000028 Rises=F Damp=F

DIIS: error= 9.28D-08 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1276.01579934600 IErMin=12 ErrMin= 9.28D-08

ErrMax= 9.28D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.46D-12 BMatP= 1.25D-11

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

Coeff-Com: 0.957D-04-0.272D-02-0.869D-03-0.298D-02 0.244D-01 0.112D+00

Coeff-Com: 0.249D-01-0.181D+00-0.161D+00-0.784D-01 0.528D+00 0.738D+00

Coeff: 0.957D-04-0.272D-02-0.869D-03-0.298D-02 0.244D-01 0.112D+00

Coeff: 0.249D-01-0.181D+00-0.161D+00-0.784D-01 0.528D+00 0.738D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.12D-08 MaxDP=5.14D-07 DE=-2.77D-11 OVMax= 7.88D-06

Cycle 13 Pass 1 IDiag 1:

RMSU= 3.30D-09 CP: 1.00D+00 1.06D+00 6.88D-01 1.71D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.80D+00 1.78D+00

CP: 1.27D+00 1.35D+00

E= -1276.01579934600 Delta-E= 0.000000000002 Rises=F Damp=F

DIIS: error= 3.90D-08 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=12 EnMin= -1276.01579934600 IErMin=13 ErrMin= 3.90D-08

ErrMax= 3.90D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.01D-12 BMatP= 6.46D-12

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

Coeff-Com: 0.754D-04-0.157D-02-0.971D-03-0.479D-02 0.311D-02 0.439D-01

Coeff-Com: 0.335D-01-0.502D-01-0.897D-01-0.133D+00 0.913D-01 0.470D+00

Coeff-Com: 0.639D+00

Coeff: 0.754D-04-0.157D-02-0.971D-03-0.479D-02 0.311D-02 0.439D-01

Coeff: 0.335D-01-0.502D-01-0.897D-01-0.133D+00 0.913D-01 0.470D+00

Coeff: 0.639D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=3.33D-09 MaxDP=1.82D-07 DE= 1.82D-12 OVMax= 2.12D-06

Error on total polarization charges = 0.06995

SCF Done: E(UB3LYP) = -1276.01579935 A.U. after 13 cycles

NFock= 13 Conv=0.33D-08 -V/T= 1.9659

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7653 S= 0.5076

<L.S>= 0.000000000000E+00

KE= 1.321002948902D+03 PE=-8.600010803991D+03 EE= 3.242809206745D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.68

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7653, after 0.7501

Leave Link 502 at Tue Sep 17 14:06:48 2019, MaxMem= 2415919104 cpu: 1270.3

(Enter /home/blab/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15317 LenP2D= 41234.

LDataN: DoStor=T MaxTD1= 6 Len= 172

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

GePol: Maximum number of non-zero 1st derivatives = 253

Leave Link 701 at Tue Sep 17 14:06:52 2019, MaxMem= 2415919104 cpu: 69.4

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 14:06:52 2019, MaxMem= 2415919104 cpu: 0.3

(Enter /home/blab/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

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

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

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

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

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Tue Sep 17 14:07:05 2019, MaxMem= 2415919104 cpu: 230.8

(Enter /home/blab/g09/l716.exe)

Dipole = 4.72510919D-13 2.63788991D-13 2.22044605D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000195359 -0.000220603 0.000000000

2 7 -0.000272136 0.000182709 -0.000000000

3 6 -0.000111345 -0.000193327 0.000000000

4 6 0.000190485 0.000010730 0.000000000

5 6 -0.000040686 0.000145099 0.000000000

6 7 0.000264069 0.000232773 0.000000000

7 6 -0.000119126 -0.000333472 -0.000000000

8 7 -0.000122902 0.000252780 0.000000000

9 6 -0.000045644 0.000118369 -0.000000000

10 6 -0.000000179 -0.000108791 0.000000000

11 6 0.000030965 0.000048188 0.000000000

12 7 -0.000123338 0.000235283 0.000000000

13 6 0.000000179 0.000108791 0.000000000

14 6 -0.000030965 -0.000048188 0.000000000

15 6 0.000119126 0.000333472 0.000000000

16 7 0.000122902 -0.000252780 0.000000000

17 6 0.000045644 -0.000118369 0.000000000

18 7 -0.000264069 -0.000232773 -0.000000000

19 7 0.000272136 -0.000182709 0.000000000

20 6 0.000111345 0.000193327 -0.000000000

21 6 -0.000190485 -0.000010730 -0.000000000

22 6 0.000040686 -0.000145099 0.000000000

23 6 -0.000195359 0.000220603 0.000000000

24 7 0.000123338 -0.000235283 0.000000000

25 30 -0.000000000 -0.000000000 0.000000000

26 6 0.000001832 0.000015271 0.000000000

27 1 0.000014851 -0.000001672 0.000000000

28 6 -0.000006794 -0.000027473 0.000000000

29 1 0.000020601 0.000014764 0.000000000

30 6 0.000006794 0.000027473 0.000000000

31 1 -0.000020601 -0.000014764 0.000000000

32 6 -0.000001832 -0.000015271 -0.000000000

33 1 -0.000014851 0.000001672 -0.000000000

34 1 0.000004905 -0.000007548 0.000000000

35 1 0.000005959 -0.000006337 0.000008065

36 1 0.000005959 -0.000006337 -0.000008065

37 1 0.000001156 0.000014733 0.000008383

38 1 0.000001156 0.000014733 -0.000008383

39 1 -0.000003603 0.000001267 0.000000000

40 1 -0.000001156 -0.000014733 0.000008383

41 1 -0.000001156 -0.000014733 -0.000008383

42 1 0.000003603 -0.000001267 0.000000000

43 1 -0.000005959 0.000006337 0.000008065

44 1 -0.000005959 0.000006337 -0.000008065

45 1 -0.000004905 0.000007548 0.000000000

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

Cartesian Forces: Max 0.000333472 RMS 0.000104428

Leave Link 716 at Tue Sep 17 14:07:05 2019, MaxMem= 2415919104 cpu: 0.3

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

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

Internal Forces: Max 0.000279871 RMS 0.000044522

Search for a local minimum.

Step number 10 out of a maximum of 270

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

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4 5

6 7 8 9 10

DE= -4.07D-06 DEPred=-3.02D-06 R= 1.35D+00

TightC=F SS= 1.41D+00 RLast= 7.33D-03 DXNew= 2.9025D-01 2.1995D-02

Trust test= 1.35D+00 RLast= 7.33D-03 DXMaxT set to 1.73D-01

ITU= 1 1 -1 1 1 1 0 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01329

Eigenvalues --- 0.01331 0.01340 0.01341 0.01608 0.01628

Eigenvalues --- 0.01636 0.01646 0.01771 0.01790 0.01804

Eigenvalues --- 0.01817 0.01887 0.01906 0.01938 0.01948

Eigenvalues --- 0.01997 0.01999 0.02045 0.02048 0.02070

Eigenvalues --- 0.02087 0.02102 0.02110 0.02114 0.02205

Eigenvalues --- 0.02313 0.02317 0.02352 0.02373 0.06920

Eigenvalues --- 0.07180 0.07180 0.07181 0.07181 0.07203

Eigenvalues --- 0.07254 0.07320 0.09453 0.13000 0.14496

Eigenvalues --- 0.14497 0.15137 0.15836 0.15993 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16001

Eigenvalues --- 0.16036 0.16509 0.17897 0.19811 0.22072

Eigenvalues --- 0.22095 0.22115 0.23775 0.23846 0.23861

Eigenvalues --- 0.24201 0.24670 0.24999 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25061

Eigenvalues --- 0.25776 0.27160 0.30410 0.33199 0.33208

Eigenvalues --- 0.33209 0.33281 0.33282 0.33282 0.33568

Eigenvalues --- 0.33721 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33724 0.33972 0.34426 0.34433

Eigenvalues --- 0.34437 0.34437 0.34689 0.35537 0.35548

Eigenvalues --- 0.35682 0.35682 0.35697 0.35731 0.37392

Eigenvalues --- 0.39368 0.41597 0.41772 0.41980 0.45464

Eigenvalues --- 0.47868 0.48965 0.48980 0.50615 0.51361

Eigenvalues --- 0.51363 0.51500 0.53605 0.54016 0.54024

Eigenvalues --- 0.54678 0.56329 0.56334 0.56767

DIIS coeff's: 1.37998 -0.24154 -0.08628 -0.01393 0.01211

DIIS coeff's: -0.09860 0.04826

Cosine: 0.944 > 0.500

Length: 1.424

GDIIS step was calculated using 7 of the last 7 vectors.

Iteration 1 RMS(Cart)= 0.00048647 RMS(Int)= 0.00000059

Iteration 2 RMS(Cart)= 0.00000033 RMS(Int)= 0.00000057

ITry= 1 IFail=0 DXMaxC= 1.94D-03 DCOld= 1.00D+10 DXMaxT= 1.73D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 2.58D-11 for atom 38.

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

(Linear) (Quad) (Total)

R1 2.58293 -0.00012 -0.00105 -0.00009 -0.00114 2.58179

R2 2.71292 -0.00007 -0.00035 -0.00001 -0.00036 2.71256

R3 2.58235 0.00017 0.00140 -0.00009 0.00131 2.58366

R4 2.58292 0.00013 0.00112 0.00009 0.00121 2.58412

R5 3.80397 -0.00004 -0.00019 0.00018 -0.00001 3.80396

R6 2.72860 -0.00014 -0.00118 -0.00002 -0.00120 2.72740

R7 2.57884 0.00009 0.00014 0.00004 0.00018 2.57902

R8 2.62371 0.00010 0.00049 0.00008 0.00058 2.62429

R9 2.82496 0.00000 0.00005 0.00001 0.00006 2.82502

R10 2.04558 -0.00001 0.00000 -0.00004 -0.00004 2.04554

R11 2.50140 -0.00028 -0.00144 -0.00011 -0.00155 2.49985

R12 2.58822 0.00013 0.00127 0.00006 0.00133 2.58955

R13 2.77746 -0.00000 0.00025 -0.00017 0.00007 2.77754

R14 2.58511 -0.00002 -0.00098 0.00014 -0.00084 2.58427

R15 3.79271 -0.00010 -0.00084 -0.00001 -0.00085 3.79186

R16 2.80242 0.00006 0.00079 0.00003 0.00082 2.80324

R17 2.49724 -0.00011 -0.00020 0.00007 -0.00013 2.49711

R18 2.56813 -0.00009 -0.00047 -0.00004 -0.00051 2.56762

R19 2.81610 -0.00001 -0.00019 0.00005 -0.00014 2.81597

R20 2.04509 -0.00000 -0.00002 0.00002 -0.00000 2.04508

R21 2.49724 -0.00011 -0.00020 0.00007 -0.00013 2.49711

R22 2.56813 -0.00009 -0.00047 -0.00004 -0.00051 2.56762

R23 2.80242 0.00006 0.00079 0.00003 0.00082 2.80324

R24 2.81610 -0.00001 -0.00019 0.00005 -0.00014 2.81597

R25 2.77746 -0.00000 0.00025 -0.00017 0.00007 2.77754

R26 2.04509 -0.00000 -0.00002 0.00002 -0.00000 2.04508

R27 2.58822 0.00013 0.00127 0.00006 0.00133 2.58955

R28 2.50140 -0.00028 -0.00144 -0.00011 -0.00155 2.49985

R29 2.58511 -0.00002 -0.00098 0.00014 -0.00084 2.58427

R30 3.79271 -0.00010 -0.00084 -0.00001 -0.00085 3.79186

R31 2.57884 0.00009 0.00014 0.00004 0.00018 2.57902

R32 2.58292 0.00013 0.00112 0.00009 0.00121 2.58412

R33 2.58293 -0.00012 -0.00105 -0.00009 -0.00114 2.58179

R34 3.80397 -0.00004 -0.00019 0.00018 -0.00001 3.80396

R35 2.72860 -0.00014 -0.00118 -0.00002 -0.00120 2.72740

R36 2.62371 0.00010 0.00049 0.00008 0.00058 2.62429

R37 2.82496 0.00000 0.00005 0.00001 0.00006 2.82502

R38 2.71292 -0.00007 -0.00035 -0.00001 -0.00036 2.71256

R39 2.04558 -0.00001 0.00000 -0.00004 -0.00004 2.04554

R40 2.58235 0.00017 0.00140 -0.00009 0.00131 2.58366

R41 2.06454 0.00000 0.00001 -0.00000 0.00001 2.06455

R42 2.07016 0.00001 -0.00000 0.00002 0.00002 2.07018

R43 2.07016 0.00001 -0.00000 0.00002 0.00002 2.07018

R44 2.06900 0.00001 0.00002 0.00004 0.00005 2.06906

R45 2.06900 0.00001 0.00002 0.00004 0.00005 2.06906

R46 2.06319 -0.00000 -0.00002 0.00001 -0.00001 2.06319

R47 2.06900 0.00001 0.00002 0.00004 0.00005 2.06906

R48 2.06900 0.00001 0.00002 0.00004 0.00005 2.06906

R49 2.06319 -0.00000 -0.00002 0.00001 -0.00001 2.06319

R50 2.07016 0.00001 -0.00000 0.00002 0.00002 2.07018

R51 2.07016 0.00001 -0.00000 0.00002 0.00002 2.07018

R52 2.06454 0.00000 0.00001 -0.00000 0.00001 2.06455

A1 1.88867 -0.00000 0.00037 -0.00007 0.00030 1.88897

A2 2.20644 -0.00006 -0.00029 -0.00006 -0.00035 2.20609

A3 2.18808 0.00006 -0.00009 0.00013 0.00005 2.18812

A4 1.90548 0.00000 -0.00026 0.00001 -0.00025 1.90522

A5 2.19150 0.00009 0.00097 0.00013 0.00109 2.19259

A6 2.18621 -0.00009 -0.00070 -0.00014 -0.00084 2.18537

A7 1.89728 0.00001 0.00004 0.00008 0.00012 1.89740

A8 2.21482 -0.00000 -0.00034 -0.00001 -0.00034 2.21448

A9 2.17108 -0.00001 0.00030 -0.00008 0.00022 2.17131

A10 1.85405 -0.00005 0.00003 -0.00017 -0.00015 1.85390

A11 2.18732 0.00002 0.00015 0.00012 0.00027 2.18759

A12 2.24182 0.00002 -0.00018 0.00005 -0.00013 2.24169

A13 1.87930 0.00003 -0.00017 0.00015 -0.00002 1.87928

A14 2.18532 -0.00001 0.00022 -0.00006 0.00016 2.18548

A15 2.21856 -0.00002 -0.00005 -0.00009 -0.00014 2.21843

A16 2.17726 0.00004 0.00089 0.00008 0.00097 2.17823

A17 2.22894 0.00001 -0.00013 0.00006 -0.00007 2.22887

A18 2.17462 -0.00002 0.00022 -0.00004 0.00018 2.17480

A19 1.87962 0.00001 -0.00009 -0.00002 -0.00011 1.87951

A20 1.91314 -0.00005 -0.00018 0.00004 -0.00014 1.91300

A21 2.18877 -0.00002 -0.00050 -0.00011 -0.00061 2.18816

A22 2.18128 0.00006 0.00068 0.00007 0.00075 2.18203

A23 1.88634 -0.00000 0.00023 -0.00013 0.00009 1.88644

A24 2.23876 0.00001 0.00056 -0.00006 0.00050 2.23926

A25 2.15809 -0.00000 -0.00079 0.00019 -0.00060 2.15749

A26 1.85872 0.00004 0.00007 0.00005 0.00012 1.85884

A27 2.16534 -0.00000 -0.00037 0.00008 -0.00029 2.16504

A28 2.25912 -0.00004 0.00030 -0.00013 0.00017 2.25930

A29 1.88695 0.00000 -0.00002 0.00006 0.00004 1.88700

A30 2.16997 0.00002 0.00005 0.00002 0.00007 2.17004

A31 2.22626 -0.00002 -0.00003 -0.00008 -0.00012 2.22615

A32 2.17717 -0.00004 -0.00114 0.00004 -0.00111 2.17607

A33 1.85872 0.00004 0.00007 0.00005 0.00012 1.85884

A34 2.25912 -0.00004 0.00030 -0.00013 0.00017 2.25930

A35 2.16534 -0.00000 -0.00037 0.00008 -0.00029 2.16504

A36 1.88695 0.00000 -0.00002 0.00006 0.00004 1.88700

A37 2.22626 -0.00002 -0.00003 -0.00008 -0.00012 2.22615

A38 2.16997 0.00002 0.00005 0.00002 0.00007 2.17004

A39 1.87962 0.00001 -0.00009 -0.00002 -0.00011 1.87951

A40 2.17462 -0.00002 0.00022 -0.00004 0.00018 2.17480

A41 2.22894 0.00001 -0.00013 0.00006 -0.00007 2.22887

A42 1.91314 -0.00005 -0.00018 0.00004 -0.00014 1.91300

A43 2.18877 -0.00002 -0.00050 -0.00011 -0.00061 2.18816

A44 2.18128 0.00006 0.00068 0.00007 0.00075 2.18203

A45 2.15809 -0.00000 -0.00079 0.00019 -0.00060 2.15749

A46 2.23876 0.00001 0.00056 -0.00006 0.00050 2.23926

A47 1.88634 -0.00000 0.00023 -0.00013 0.00009 1.88644

A48 2.17726 0.00004 0.00089 0.00008 0.00097 2.17823

A49 1.90548 0.00000 -0.00026 0.00001 -0.00025 1.90522

A50 2.18621 -0.00009 -0.00070 -0.00014 -0.00084 2.18537

A51 2.19150 0.00009 0.00097 0.00013 0.00109 2.19259

A52 2.21482 -0.00000 -0.00034 -0.00001 -0.00034 2.21448

A53 2.17108 -0.00001 0.00030 -0.00008 0.00022 2.17131

A54 1.89728 0.00001 0.00004 0.00008 0.00012 1.89740

A55 1.85405 -0.00005 0.00003 -0.00017 -0.00015 1.85390

A56 2.18732 0.00002 0.00015 0.00012 0.00027 2.18759

A57 2.24182 0.00002 -0.00018 0.00005 -0.00013 2.24169

A58 1.87930 0.00003 -0.00017 0.00015 -0.00002 1.87928

A59 2.21856 -0.00002 -0.00005 -0.00009 -0.00014 2.21843

A60 2.18532 -0.00001 0.00022 -0.00006 0.00016 2.18548

A61 1.88867 -0.00000 0.00037 -0.00007 0.00030 1.88897

A62 2.20644 -0.00006 -0.00029 -0.00006 -0.00035 2.20609

A63 2.18808 0.00006 -0.00009 0.00013 0.00005 2.18812

A64 2.17717 -0.00004 -0.00114 0.00004 -0.00111 2.17607

A65 1.57037 0.00006 0.00078 0.00011 0.00089 1.57127

A66 1.57122 -0.00006 -0.00078 -0.00011 -0.00089 1.57033

A67 1.57122 -0.00006 -0.00078 -0.00011 -0.00089 1.57033

A68 1.57037 0.00006 0.00078 0.00011 0.00089 1.57127

A69 1.94200 0.00000 0.00017 -0.00011 0.00006 1.94206

A70 1.94961 0.00000 0.00007 -0.00000 0.00007 1.94968

A71 1.94961 0.00000 0.00007 -0.00000 0.00007 1.94968

A72 1.88072 -0.00001 -0.00012 0.00001 -0.00011 1.88061

A73 1.88072 -0.00001 -0.00012 0.00001 -0.00011 1.88061

A74 1.85705 -0.00000 -0.00009 0.00009 0.00001 1.85705

A75 1.93977 0.00000 -0.00006 0.00004 -0.00002 1.93975

A76 1.93977 0.00000 -0.00006 0.00004 -0.00002 1.93975

A77 1.94558 -0.00001 0.00020 -0.00015 0.00005 1.94563

A78 1.85741 -0.00000 -0.00020 0.00006 -0.00014 1.85728

A79 1.88902 0.00000 0.00005 0.00001 0.00006 1.88909

A80 1.88902 0.00000 0.00005 0.00001 0.00006 1.88909

A81 1.93977 0.00000 -0.00006 0.00004 -0.00002 1.93975

A82 1.93977 0.00000 -0.00006 0.00004 -0.00002 1.93975

A83 1.94558 -0.00001 0.00020 -0.00015 0.00005 1.94563

A84 1.85741 -0.00000 -0.00020 0.00006 -0.00014 1.85728

A85 1.88902 0.00000 0.00005 0.00001 0.00006 1.88909

A86 1.88902 0.00000 0.00005 0.00001 0.00006 1.88909

A87 1.94961 0.00000 0.00007 -0.00000 0.00007 1.94968

A88 1.94961 0.00000 0.00007 -0.00000 0.00007 1.94968

A89 1.94200 0.00000 0.00017 -0.00011 0.00006 1.94206

A90 1.85705 -0.00000 -0.00009 0.00009 0.00001 1.85705

A91 1.88072 -0.00001 -0.00012 0.00001 -0.00011 1.88061

A92 1.88072 -0.00001 -0.00012 0.00001 -0.00011 1.88061

A93 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

A94 3.14159 0.00000 -0.00000 -0.00000 0.00000 3.14159

A95 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

A96 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D1 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D2 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D3 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D4 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D5 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D6 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D7 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D8 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D9 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D10 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D11 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D12 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

D13 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D14 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D15 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D16 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D17 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D18 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

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D125 1.03888 0.00000 -0.00001 0.00006 0.00005 1.03893

D126 -1.03888 -0.00000 0.00001 -0.00006 -0.00005 -1.03893

D127 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D128 -2.10271 0.00000 -0.00001 0.00006 0.00005 -2.10266

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Item Value Threshold Converged?

Maximum Force 0.000280 0.000450 YES

RMS Force 0.000045 0.000300 YES

Maximum Displacement 0.001936 0.001800 NO

RMS Displacement 0.000486 0.001200 YES

Predicted change in Energy=-1.012359D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:07:05 2019, MaxMem= 2415919104 cpu: 1.1

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.074998 -2.194745 -0.000000

2 7 0 -0.748240 -1.868735 -0.000000

3 6 0 -0.004140 -3.016019 -0.000000

4 6 0 -0.899058 -4.148349 -0.000000

5 6 0 -2.185745 -3.625892 -0.000000

6 7 0 1.357438 -3.109171 -0.000000

7 6 0 2.184855 -2.077015 -0.000000

8 7 0 1.863145 -0.744985 -0.000000

9 6 0 3.007653 0.003518 -0.000000

10 6 0 4.164855 -0.924592 -0.000000

11 6 0 3.650885 -2.182357 -0.000000

12 7 0 -3.125480 -1.319668 -0.000000

13 6 0 -4.164855 0.924592 -0.000000

14 6 0 -3.650885 2.182357 -0.000000

15 6 0 -2.184855 2.077015 -0.000000

16 7 0 -1.863145 0.744985 -0.000000

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25 30 0 0.000000 -0.000000 -0.000000

26 6 0 -0.478478 -5.582904 -0.000000

27 1 0 -3.115587 -4.180055 -0.000000

28 6 0 5.588193 -0.483411 -0.000000

29 1 0 4.195655 -3.117454 -0.000000

30 6 0 -5.588193 0.483411 -0.000000

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34 1 0 -1.343927 -6.249676 -0.000000

35 1 0 0.130841 -5.826522 0.877204

36 1 0 0.130841 -5.826522 -0.877204

37 1 0 5.810342 0.133576 0.876799

38 1 0 5.810342 0.133576 -0.876799

39 1 0 6.270796 -1.335504 -0.000000

40 1 0 -5.810342 -0.133576 0.876799

41 1 0 -5.810342 -0.133576 -0.876799

42 1 0 -6.270796 1.335504 -0.000000

43 1 0 -0.130841 5.826522 0.877204

44 1 0 -0.130841 5.826522 -0.877204

45 1 0 1.343927 6.249676 -0.000000

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Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.366225 0.000000

3 C 2.227767 1.367459 0.000000

4 C 2.280220 2.284598 1.443278 0.000000

5 C 1.435425 2.270247 2.265247 1.388714 0.000000

6 N 3.552153 2.443883 1.364761 2.484284 3.580663

7 C 4.261480 2.940481 2.381896 3.714962 4.636934

8 N 4.196520 2.842912 2.940128 4.383224 4.969219

9 C 5.537663 4.196673 4.264798 5.700912 6.335929

10 C 6.367814 5.002990 4.664181 6.002984 6.901242

11 C 5.725896 4.410290 3.748893 4.956521 6.012490

12 N 1.367213 2.439824 3.552516 3.599777 2.490336

13 C 3.754699 4.413155 5.730616 6.033255 4.962236

14 C 4.652143 4.983642 6.349949 6.902926 5.990191

15 C 4.273173 4.199144 5.540263 6.356763 5.702908

16 N 2.947354 2.841574 4.195360 4.987402 4.382766

17 C 2.381453 2.929843 4.253969 4.650355 3.714448

18 N 5.352235 5.015044 6.272907 7.271981 6.785806

19 N 4.947984 4.025933 4.942357 6.238501 6.228900

20 C 5.610247 4.942357 6.032043 7.221076 6.993610

21 C 7.005702 6.238501 7.221076 8.489312 8.363901

22 C 7.213442 6.228900 6.993610 8.363901 8.467484

23 C 6.040703 4.947984 5.610247 7.005702 7.213442

24 N 6.276628 5.017132 5.347214 6.789411 7.257249

25 Zn 3.020352 2.012966 3.016022 4.244656 4.233742

26 C 3.745464 3.723953 2.610344 1.494936 2.597047

27 H 2.241491 3.308555 3.322060 2.216756 1.082453

28 C 7.851953 6.486101 6.139079 7.450919 8.385064

29 H 6.338177 5.099157 4.201020 5.197965 6.401623

30 C 4.417585 5.381239 6.589966 6.590994 5.335075

31 H 5.719847 6.061910 7.428882 7.978687 7.036509

32 C 8.186090 7.551938 8.612456 9.828270 9.586449

33 H 8.220721 7.177536 7.843225 9.245523 9.435939

34 H 4.120307 4.421254 3.500224 2.147902 2.755522

35 H 4.338781 4.148054 2.947310 2.155561 3.313432

36 H 4.338781 4.148054 2.947310 2.155561 3.313432

37 H 8.268521 6.913250 6.670601 8.007478 8.879177

38 H 8.268521 6.913250 6.670601 8.007478 8.879177

39 H 8.389910 7.039262 6.496073 7.701877 8.761219

40 H 4.355455 5.422585 6.541348 6.403741 5.109085

41 H 4.355455 5.422585 6.541348 6.403741 5.109085

42 H 5.483373 6.384808 7.629334 7.676472 6.426749

43 H 8.299998 7.769663 8.886848 10.042794 9.712891

44 H 8.299998 7.769663 8.886848 10.042794 9.712891

45 H 9.110285 8.383660 9.363246 10.637195 10.487394

6 7 8 9 10

6 N 0.000000

7 C 1.322862 0.000000

8 N 2.417668 1.370330 0.000000

9 C 3.523073 2.237324 1.367536 0.000000

10 C 3.557242 2.290956 2.308707 1.483410 0.000000

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12 N 4.826891 5.364068 5.021617 6.274244 7.301031

13 C 6.838638 7.023423 6.254940 7.231407 8.532500

14 C 7.285847 7.224826 6.242904 7.005959 8.410643

15 C 6.280475 6.029124 4.934571 5.591201 7.023423

16 N 5.022616 4.934571 4.013134 4.926910 6.254940

17 C 5.357154 5.591201 4.926910 6.015310 7.231407

18 N 6.785155 6.280475 5.022616 5.357154 6.838638

19 N 5.015044 4.199144 2.841574 2.929843 4.413155

20 C 6.272907 5.540263 4.195360 4.253969 5.730616

21 C 7.271981 6.356763 4.987402 4.650355 6.033255

22 C 6.785806 5.702908 4.382766 3.714448 4.962236

23 C 5.352235 4.273173 2.947354 2.381453 3.754699

24 N 4.768708 3.524518 2.419975 1.321413 2.473258

25 Zn 3.392577 3.014562 2.006567 3.007655 4.266250

26 C 3.080575 4.402794 5.374818 6.584924 6.577265

27 H 4.599429 5.702409 6.048759 7.415953 7.975141

28 C 4.979347 3.757963 3.734220 2.626078 1.490145

29 H 2.838229 2.264029 3.327043 3.339434 2.193078

30 C 7.819747 8.183890 7.551913 8.609231 9.854157

31 H 8.343123 8.227601 7.185227 7.847563 9.286348

32 C 8.736403 7.847680 6.477614 6.125869 7.479096

33 H 7.498260 6.325915 5.081794 4.177931 5.211371

34 H 4.142480 5.464741 6.370788 7.618313 7.661801

35 H 3.107737 4.364317 5.439889 6.560100 6.408718

36 H 3.107737 4.364317 5.439889 6.560100 6.408718

37 H 5.577861 4.335856 4.137754 2.939516 2.143857

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39 H 5.223695 4.152681 4.447033 3.527192 2.145656

40 H 7.810251 8.274594 7.747580 8.862539 10.044851

41 H 7.810251 8.274594 7.747580 8.862539 10.044851

42 H 8.828652 9.118297 8.395799 9.373570 10.677587

43 H 9.101158 8.282382 6.923162 6.672856 8.049847

44 H 9.101158 8.282382 6.923162 6.672856 8.049847

45 H 9.358857 8.369047 7.013905 6.463936 7.708941

11 12 13 14 15

11 C 0.000000

12 N 6.831057 0.000000

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16 N 6.242904 2.419975 2.308707 2.293916 1.370330

17 C 7.005959 1.321413 1.483410 2.278551 2.237324

18 N 7.285847 4.768708 3.557242 2.473637 1.322862

19 N 4.983642 5.017132 5.002990 4.410290 2.940481

20 C 6.349949 5.347214 4.664181 3.748893 2.381896

21 C 6.902926 6.789411 6.002984 4.956521 3.714962

22 C 5.990191 7.257249 6.901242 6.012490 4.636934

23 C 4.652143 6.276628 6.367814 5.725896 4.261480

24 N 3.541218 6.785321 7.301031 6.831057 5.364068

25 Zn 4.253427 3.392660 4.266250 4.253427 3.014562

26 C 5.349333 5.018147 7.479096 8.388292 7.847680

27 H 7.055207 2.860405 5.211371 6.384891 6.325915

28 C 2.576738 8.753708 9.854157 9.615970 8.183890

29 H 1.082212 7.538637 9.286348 9.468695 8.227601

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32 C 8.388292 7.786784 6.577265 5.349333 4.402794

33 H 6.384891 8.318526 7.975141 7.055207 5.702409

34 H 6.441369 5.242034 7.708941 8.741924 8.369047

35 H 5.141998 5.628930 8.049847 8.900173 8.282382

36 H 5.141998 5.628930 8.049847 8.900173 8.282382

37 H 3.285662 9.095581 10.044851 9.720138 8.274594

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39 H 2.753379 9.396289 10.677587 10.526875 9.118297

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42 H 10.526875 4.116182 2.145656 2.753379 4.152681

43 H 8.900173 7.797780 6.408718 5.141998 4.364317

44 H 8.900173 7.797780 6.408718 5.141998 4.364317

45 H 8.741924 8.790367 7.661801 6.441369 5.464741

16 17 18 19 20

16 N 0.000000

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18 N 2.417668 3.523073 0.000000

19 N 2.842912 4.196673 2.443883 0.000000

20 C 2.940128 4.264798 1.364761 1.367459 0.000000

21 C 4.383224 5.700912 2.484284 2.284598 1.443278

22 C 4.969219 6.335929 3.580663 2.270247 2.265247

23 C 4.196520 5.537663 3.552153 1.366225 2.227767

24 N 5.021617 6.274244 4.826891 2.439824 3.552516

25 Zn 2.006567 3.007655 3.392577 2.012966 3.016022

26 C 6.477614 6.125869 8.736403 7.551938 8.612456

27 H 5.081794 4.177931 7.498260 7.177536 7.843225

28 C 7.551913 8.609231 7.819747 5.381239 6.589966

29 H 7.185227 7.847563 8.343123 6.061910 7.428882

30 C 3.734220 2.626078 4.979347 6.486101 6.139079

31 H 3.327043 3.339434 2.838229 5.099157 4.201020

32 C 5.374818 6.584924 3.080575 3.723953 2.610344

33 H 6.048759 7.415953 4.599429 3.308555 3.322060

34 H 7.013905 6.463936 9.358857 8.383660 9.363246

35 H 6.923162 6.672856 9.101158 7.769663 8.886848

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37 H 7.747580 8.862539 7.810251 5.422585 6.541348

38 H 7.747580 8.862539 7.810251 5.422585 6.541348

39 H 8.395799 9.373570 8.828652 6.384808 7.629334

40 H 4.137754 2.939516 5.577861 6.913250 6.670601

41 H 4.137754 2.939516 5.577861 6.913250 6.670601

42 H 4.447033 3.527192 5.223695 7.039262 6.496073

43 H 5.439889 6.560100 3.107737 4.148054 2.947310

44 H 5.439889 6.560100 3.107737 4.148054 2.947310

45 H 6.370788 7.618313 4.142480 4.421254 3.500224

21 22 23 24 25

21 C 0.000000

22 C 1.388714 0.000000

23 C 2.280220 1.435425 0.000000

24 N 3.599777 2.490336 1.367213 0.000000

25 Zn 4.244656 4.233742 3.020352 3.392660 0.000000

26 C 9.828270 9.586449 8.186090 7.786784 5.603370

27 H 9.245523 9.435939 8.220721 8.318526 5.213420

28 C 6.590994 5.335075 4.417585 3.052221 5.609063

29 H 7.978687 7.036509 5.719847 4.564354 5.227049

30 C 7.450919 8.385064 7.851953 8.753708 5.609063

31 H 5.197965 6.401623 6.338177 7.538637 5.227049

32 C 1.494936 2.597047 3.745464 5.018147 5.603370

33 H 2.216756 1.082453 2.241491 2.860405 5.213420

34 H 10.637195 10.487394 9.110285 8.790367 6.392542

35 H 10.042794 9.712891 8.299998 7.797780 5.893638

36 H 10.042794 9.712891 8.299998 7.797780 5.893638

37 H 6.403741 5.109085 4.355455 3.063344 5.877643

38 H 6.403741 5.109085 4.355455 3.063344 5.877643

39 H 7.676472 6.426749 5.483373 4.116182 6.411432

40 H 8.007478 8.879177 8.268521 9.095581 5.877643

41 H 8.007478 8.879177 8.268521 9.095581 5.877643

42 H 7.701877 8.761219 8.389910 9.396289 6.411432

43 H 2.155561 3.313432 4.338781 5.628930 5.893638

44 H 2.155561 3.313432 4.338781 5.628930 5.893638

45 H 2.147902 2.755522 4.120307 5.242034 6.392542

26 27 28 29 30

26 C 0.000000

27 H 2.987027 0.000000

28 C 7.925234 9.456266 0.000000

29 H 5.284502 7.388057 2.979487 0.000000

30 C 7.931542 5.278418 11.218126 10.425445 0.000000

31 H 9.461165 7.377004 10.425445 10.454098 2.979487

32 C 11.206741 10.403494 7.931542 9.461165 7.925234

33 H 10.403494 10.426840 5.278418 7.377004 9.456266

34 H 1.092514 2.724355 9.016878 6.363787 7.959162

35 H 1.095494 3.744281 7.687718 4.962988 8.561081

36 H 1.095494 3.744281 7.687718 4.962988 8.561081

37 H 8.543780 9.952306 1.094897 3.734325 11.437559

38 H 8.543780 9.952306 1.094897 3.734325 11.437559

39 H 7.974529 9.807939 1.091792 2.735244 11.997670

40 H 7.674160 4.940089 11.437559 10.478181 1.094897

41 H 7.674160 4.940089 11.437559 10.478181 1.094897

42 H 9.023044 6.354269 11.997670 11.374333 1.091792

43 H 11.448378 10.479017 8.561081 9.974105 7.687718

44 H 11.448378 10.479017 8.561081 9.974105 7.687718

45 H 11.972097 11.343129 7.959162 9.791603 9.016878

31 32 33 34 35

31 H 0.000000

32 C 5.284502 0.000000

33 H 7.388057 2.987027 0.000000

34 H 9.791603 11.972097 11.343129 0.000000

35 H 9.974105 11.448378 10.479017 1.767339 0.000000

36 H 9.974105 11.448378 10.479017 1.767339 1.754408

37 H 10.478181 7.674160 4.940089 9.627992 8.232831

38 H 10.478181 7.674160 4.940089 9.627992 8.417602

39 H 11.374333 9.023044 6.354269 9.062731 7.657531

40 H 3.734325 8.543780 9.952306 7.623931 8.228444

41 H 3.734325 8.543780 9.952306 7.623931 8.413312

42 H 2.735244 7.974529 9.807939 9.044833 9.645987

43 H 4.962988 1.095494 3.744281 12.168633 11.655983

44 H 4.962988 1.095494 3.744281 12.168633 11.787276

45 H 6.363787 1.092514 2.724355 12.785084 12.168633

36 37 38 39 40

36 H 0.000000

37 H 8.417602 0.000000

38 H 8.232831 1.753598 0.000000

39 H 7.657531 1.771720 1.771720 0.000000

40 H 8.413312 11.623754 11.755287 12.172400 0.000000

41 H 8.228444 11.755287 11.623754 12.172400 1.753598

42 H 9.645987 12.172400 12.172400 12.822864 1.771720

43 H 11.787276 8.228444 8.413312 9.645987 8.232831

44 H 11.655983 8.413312 8.228444 9.645987 8.417602

45 H 12.168633 7.623931 7.623931 9.044833 9.627992

41 42 43 44 45

41 H 0.000000

42 H 1.771720 0.000000

43 H 8.417602 7.657531 0.000000

44 H 8.232831 7.657531 1.754408 0.000000

45 H 9.627992 9.062731 1.767339 1.767339 0.000000

Stoichiometry C20H16N8Zn(1-,2)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=3 Diff= 1.11D-04

Largest Abelian subgroup C2H NOp 4

Largest concise Abelian subgroup C2H NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.948481 0.654969 0.000000

2 7 0 -1.987918 -0.316570 0.000000

3 6 0 -2.590893 -1.543911 0.000000

4 6 0 -4.021983 -1.356746 0.000000

5 6 0 -4.233713 0.015731 0.000000

6 7 0 -1.972248 -2.760402 0.000000

7 6 0 -0.661775 -2.941027 0.000000

8 7 0 0.316496 -1.981449 0.000000

9 6 0 1.546193 -2.579782 0.000000

10 6 0 1.343298 -4.049252 0.000000

11 6 0 0.000000 -4.253427 0.000000

12 7 0 -2.736350 2.005625 0.000000

13 6 0 -1.343298 4.049252 0.000000

14 6 0 0.000000 4.253427 0.000000

15 6 0 0.661775 2.941027 0.000000

16 7 0 -0.316496 1.981449 0.000000

17 6 0 -1.546193 2.579782 0.000000

18 7 0 1.972248 2.760402 0.000000

19 7 0 1.987918 0.316570 0.000000

20 6 0 2.590893 1.543911 0.000000

21 6 0 4.021983 1.356746 0.000000

22 6 0 4.233713 -0.015731 0.000000

23 6 0 2.948481 -0.654969 0.000000

24 7 0 2.736350 -2.005625 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -5.037526 -2.453791 0.000000

27 1 0 -5.186459 0.529521 0.000000

28 6 0 2.452270 -5.044597 0.000000

29 1 0 -0.523119 -5.200806 0.000000

30 6 0 -2.452270 5.044597 0.000000

31 1 0 0.523119 5.200806 0.000000

32 6 0 5.037526 2.453791 0.000000

33 1 0 5.186459 -0.529521 0.000000

34 1 0 -6.053889 -2.053051 0.000000

35 1 0 -4.934003 -3.101790 0.877204

36 1 0 -4.934003 -3.101790 -0.877204

37 1 0 3.095835 -4.918711 0.876799

38 1 0 3.095835 -4.918711 -0.876799

39 1 0 2.071117 -6.067696 0.000000

40 1 0 -3.095835 4.918711 0.876799

41 1 0 -3.095835 4.918711 -0.876799

42 1 0 -2.071117 6.067696 0.000000

43 1 0 4.934003 3.101790 0.877204

44 1 0 4.934003 3.101790 -0.877204

45 1 0 6.053889 2.053051 0.000000

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

Rotational constants (GHZ): 0.1827855 0.1817031 0.0913256

Leave Link 202 at Tue Sep 17 14:07:05 2019, MaxMem= 2415919104 cpu: 0.2

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 229 symmetry adapted cartesian basis functions of AG symmetry.

There are 82 symmetry adapted cartesian basis functions of BG symmetry.

There are 78 symmetry adapted cartesian basis functions of AU symmetry.

There are 218 symmetry adapted cartesian basis functions of BU symmetry.

There are 212 symmetry adapted basis functions of AG symmetry.

There are 82 symmetry adapted basis functions of BG symmetry.

There are 78 symmetry adapted basis functions of AU symmetry.

There are 204 symmetry adapted basis functions of BU symmetry.

576 basis functions, 1015 primitive gaussians, 607 cartesian basis functions

103 alpha electrons 102 beta electrons

nuclear repulsion energy 2760.3921474032 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= 45 NActive= 45 NUniq= 21 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1141615085 Hartrees.

Nuclear repulsion after empirical dispersion term = 2760.2779858947 Hartrees.

No density basis found on file 724.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

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 = 45

GePol: Total number of spheres = 45

GePol: Number of exposed spheres = 45 (100.00%)

GePol: Number of points = 3614

GePol: Average weight of points = 0.10

GePol: Minimum weight of points = 0.37D-10

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 282

GePol: Fraction of low-weight points (<1% of avg) = 7.80%

GePol: Cavity surface area = 378.813 Ang\*\*2

GePol: Cavity volume = 378.205 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0106440925 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2760.2673418022 Hartrees.

Leave Link 301 at Tue Sep 17 14:07:05 2019, MaxMem= 2415919104 cpu: 1.7

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15317 LenP2D= 41234.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.79D-04 NBF= 212 82 78 204

NBsUse= 576 1.00D-06 EigRej= -1.00D+00 NBFU= 212 82 78 204

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= 594 594 594 594 594 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Tue Sep 17 14:07:06 2019, MaxMem= 2415919104 cpu: 10.4

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:07:06 2019, MaxMem= 2415919104 cpu: 1.2

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

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

B after Tr= -0.000000 -0.000000 -0.000000

Rot= 1.000000 -0.000000 0.000000 -0.000032 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-BG.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7653 S= 0.5076

Leave Link 401 at Tue Sep 17 14:07:07 2019, MaxMem= 2415919104 cpu: 20.3

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1141655 IEndB= 1141655 NGot= 2415919104 MDV= 2415163146

LenX= 2415163146 LenY= 2414794090

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= 670000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 39182988.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.77D-15 for 3598.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.60D-15 for 3001 2705.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.22D-15 for 3598.

Iteration 1 A^-1\*A deviation from orthogonality is 1.55D-12 for 1972 1970.

E= -1276.01579374112

DIIS: error= 6.79D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1276.01579374112 IErMin= 1 ErrMin= 6.79D-05

ErrMax= 6.79D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.59D-05 BMatP= 1.59D-05

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

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 0.294 Goal= None Shift= 0.000

Gap= 0.343 Goal= None Shift= 0.000

RMSDP=6.36D-06 MaxDP=1.71D-04 OVMax= 1.58D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 6.36D-06 CP: 1.00D+00

E= -1276.01579910978 Delta-E= -0.000005368660 Rises=F Damp=F

DIIS: error= 4.96D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1276.01579910978 IErMin= 2 ErrMin= 4.96D-05

ErrMax= 4.96D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.37D-06 BMatP= 1.59D-05

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

Coeff-Com: 0.905D-01 0.910D+00

Coeff: 0.905D-01 0.910D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=2.91D-06 MaxDP=1.40D-04 DE=-5.37D-06 OVMax= 1.78D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.89D-06 CP: 1.00D+00 1.05D+00

E= -1276.01579880920 Delta-E= 0.000000300572 Rises=F Damp=F

DIIS: error= 8.02D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1276.01579910978 IErMin= 2 ErrMin= 4.96D-05

ErrMax= 8.02D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.71D-06 BMatP= 1.37D-06

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

Coeff-Com: -0.158D-01 0.639D+00 0.377D+00

Coeff: -0.158D-01 0.639D+00 0.377D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.68D-06 MaxDP=7.04D-05 DE= 3.01D-07 OVMax= 2.98D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.17D-06 CP: 1.00D+00 1.15D+00 6.33D-01

E= -1276.01579966930 Delta-E= -0.000000860092 Rises=F Damp=F

DIIS: error= 1.82D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1276.01579966930 IErMin= 4 ErrMin= 1.82D-05

ErrMax= 1.82D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.29D-08 BMatP= 1.37D-06

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

Coeff-Com: -0.964D-02 0.159D+00 0.108D+00 0.742D+00

Coeff: -0.964D-02 0.159D+00 0.108D+00 0.742D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=8.67D-07 MaxDP=4.58D-05 DE=-8.60D-07 OVMax= 6.66D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.51D-07 CP: 1.00D+00 1.18D+00 8.65D-01 1.33D+00

E= -1276.01579974915 Delta-E= -0.000000079850 Rises=F Damp=F

DIIS: error= 1.40D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1276.01579974915 IErMin= 5 ErrMin= 1.40D-05

ErrMax= 1.40D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.14D-08 BMatP= 5.29D-08

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

Coeff-Com: -0.445D-03 0.786D-03-0.427D-01 0.304D+00 0.739D+00

Coeff: -0.445D-03 0.786D-03-0.427D-01 0.304D+00 0.739D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=7.61D-07 MaxDP=3.56D-05 DE=-7.99D-08 OVMax= 5.92D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.82D-07 CP: 1.00D+00 1.22D+00 1.01D+00 1.76D+00 1.40D+00

E= -1276.01579981223 Delta-E= -0.000000063082 Rises=F Damp=F

DIIS: error= 1.05D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1276.01579981223 IErMin= 6 ErrMin= 1.05D-05

ErrMax= 1.05D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.96D-08 BMatP= 4.14D-08

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

Coeff-Com: 0.917D-02-0.142D+00-0.197D+00-0.531D+00 0.432D+00 0.143D+01

Coeff: 0.917D-02-0.142D+00-0.197D+00-0.531D+00 0.432D+00 0.143D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.76D-06 MaxDP=8.70D-05 DE=-6.31D-08 OVMax= 1.38D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.51D-07 CP: 1.00D+00 1.31D+00 1.39D+00 2.74D+00 2.74D+00

CP: 2.24D+00

E= -1276.01579991435 Delta-E= -0.000000102125 Rises=F Damp=F

DIIS: error= 5.44D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1276.01579991435 IErMin= 7 ErrMin= 5.44D-06

ErrMax= 5.44D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.91D-09 BMatP= 2.96D-08

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

Coeff-Com: 0.403D-02-0.394D-01-0.707D-01-0.364D+00-0.239D+00 0.423D+00

Coeff-Com: 0.129D+01

Coeff: 0.403D-02-0.394D-01-0.707D-01-0.364D+00-0.239D+00 0.423D+00

Coeff: 0.129D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.52D-06 MaxDP=7.53D-05 DE=-1.02D-07 OVMax= 1.19D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 7.74D-07 CP: 1.00D+00 1.38D+00 1.71D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.72D+00

E= -1276.01579995146 Delta-E= -0.000000037107 Rises=F Damp=F

DIIS: error= 1.58D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1276.01579995146 IErMin= 8 ErrMin= 1.58D-06

ErrMax= 1.58D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.82D-09 BMatP= 7.91D-09

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

Coeff-Com: -0.966D-03 0.320D-01 0.284D-01-0.171D-01-0.284D+00-0.231D+00

Coeff-Com: 0.788D+00 0.685D+00

Coeff: -0.966D-03 0.320D-01 0.284D-01-0.171D-01-0.284D+00-0.231D+00

Coeff: 0.788D+00 0.685D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=3.80D-07 MaxDP=1.93D-05 DE=-3.71D-08 OVMax= 2.91D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 5.98D-08 CP: 1.00D+00 1.40D+00 1.79D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.08D+00 1.35D+00

E= -1276.01579995384 Delta-E= -0.000000002380 Rises=F Damp=F

DIIS: error= 7.99D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1276.01579995384 IErMin= 9 ErrMin= 7.99D-07

ErrMax= 7.99D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.06D-10 BMatP= 2.82D-09

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

Coeff-Com: -0.117D-02 0.211D-01 0.288D-01 0.672D-01-0.702D-01-0.149D+00

Coeff-Com: 0.371D-01 0.283D+00 0.783D+00

Coeff: -0.117D-02 0.211D-01 0.288D-01 0.672D-01-0.702D-01-0.149D+00

Coeff: 0.371D-01 0.283D+00 0.783D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=3.58D-08 MaxDP=2.68D-06 DE=-2.38D-09 OVMax= 1.32D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 3.28D-08 CP: 1.00D+00 1.40D+00 1.79D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.16D+00 1.35D+00 1.06D+00

E= -1276.01579995415 Delta-E= -0.000000000307 Rises=F Damp=F

DIIS: error= 3.70D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1276.01579995415 IErMin=10 ErrMin= 3.70D-07

ErrMax= 3.70D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.60D-10 BMatP= 5.06D-10

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

Coeff-Com: -0.409D-03 0.325D-02 0.884D-02 0.435D-01 0.378D-01-0.100D-01

Coeff-Com: -0.184D+00-0.260D-01 0.396D+00 0.731D+00

Coeff: -0.409D-03 0.325D-02 0.884D-02 0.435D-01 0.378D-01-0.100D-01

Coeff: -0.184D+00-0.260D-01 0.396D+00 0.731D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=6.32D-08 MaxDP=2.78D-06 DE=-3.07D-10 OVMax= 4.76D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.77D-08 CP: 1.00D+00 1.39D+00 1.78D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.17D+00 1.29D+00 1.12D+00 1.36D+00

E= -1276.01579995423 Delta-E= -0.000000000079 Rises=F Damp=F

DIIS: error= 1.98D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1276.01579995423 IErMin=11 ErrMin= 1.98D-07

ErrMax= 1.98D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.49D-11 BMatP= 1.60D-10

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

Coeff-Com: 0.221D-03-0.658D-02-0.658D-02-0.240D-02 0.452D-01 0.475D-01

Coeff-Com: -0.107D+00-0.116D+00-0.791D-01 0.402D+00 0.823D+00

Coeff: 0.221D-03-0.658D-02-0.658D-02-0.240D-02 0.452D-01 0.475D-01

Coeff: -0.107D+00-0.116D+00-0.791D-01 0.402D+00 0.823D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.63D-08 MaxDP=1.16D-06 DE=-7.87D-11 OVMax= 6.72D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 7.78D-09 CP: 1.00D+00 1.39D+00 1.78D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.19D+00 1.29D+00 1.18D+00 1.68D+00

CP: 1.24D+00

E= -1276.01579995427 Delta-E= -0.000000000044 Rises=F Damp=F

DIIS: error= 1.17D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1276.01579995427 IErMin=12 ErrMin= 1.17D-07

ErrMax= 1.17D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.73D-11 BMatP= 4.49D-11

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

Coeff-Com: 0.222D-03-0.447D-02-0.624D-02-0.108D-01 0.180D-01 0.245D-01

Coeff-Com: -0.182D-01-0.610D-01-0.139D+00 0.743D-01 0.463D+00 0.659D+00

Coeff: 0.222D-03-0.447D-02-0.624D-02-0.108D-01 0.180D-01 0.245D-01

Coeff: -0.182D-01-0.610D-01-0.139D+00 0.743D-01 0.463D+00 0.659D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.48D-08 MaxDP=7.64D-07 DE=-4.41D-11 OVMax= 1.05D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 3.85D-09 CP: 1.00D+00 1.39D+00 1.78D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.20D+00 1.30D+00 1.21D+00 1.78D+00

CP: 1.37D+00 1.14D+00

E= -1276.01579995430 Delta-E= -0.000000000030 Rises=F Damp=F

DIIS: error= 7.52D-08 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1276.01579995430 IErMin=13 ErrMin= 7.52D-08

ErrMax= 7.52D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.94D-12 BMatP= 1.73D-11

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

Coeff-Com: 0.366D-04 0.570D-04-0.120D-02-0.330D-02-0.386D-02-0.782D-02

Coeff-Com: 0.245D-01 0.660D-02-0.440D-01-0.774D-01-0.483D-01 0.279D+00

Coeff-Com: 0.875D+00

Coeff: 0.366D-04 0.570D-04-0.120D-02-0.330D-02-0.386D-02-0.782D-02

Coeff: 0.245D-01 0.660D-02-0.440D-01-0.774D-01-0.483D-01 0.279D+00

Coeff: 0.875D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.43D-08 MaxDP=6.74D-07 DE=-2.96D-11 OVMax= 1.09D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 1.85D-09 CP: 1.00D+00 1.39D+00 1.78D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.21D+00 1.31D+00 1.24D+00 1.82D+00

CP: 1.41D+00 1.39D+00 1.30D+00

E= -1276.01579995428 Delta-E= 0.000000000015 Rises=F Damp=F

DIIS: error= 3.06D-08 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=13 EnMin= -1276.01579995430 IErMin=14 ErrMin= 3.06D-08

ErrMax= 3.06D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.85D-13 BMatP= 3.94D-12

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

Coeff-Com: -0.158D-04 0.772D-03 0.313D-03-0.189D-03-0.512D-02-0.944D-02

Coeff-Com: 0.169D-01 0.146D-01-0.158D-02-0.521D-01-0.102D+00 0.340D-01

Coeff-Com: 0.471D+00 0.633D+00

Coeff: -0.158D-04 0.772D-03 0.313D-03-0.189D-03-0.512D-02-0.944D-02

Coeff: 0.169D-01 0.146D-01-0.158D-02-0.521D-01-0.102D+00 0.340D-01

Coeff: 0.471D+00 0.633D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=7.11D-09 MaxDP=3.34D-07 DE= 1.46D-11 OVMax= 5.53D-06

Error on total polarization charges = 0.06995

SCF Done: E(UB3LYP) = -1276.01579995 A.U. after 14 cycles

NFock= 14 Conv=0.71D-08 -V/T= 1.9659

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7652 S= 0.5076

<L.S>= 0.000000000000E+00

KE= 1.321005085480D+03 PE=-8.600184223223D+03 EE= 3.242895995986D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.68

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7652, after 0.7501

Leave Link 502 at Tue Sep 17 14:08:24 2019, MaxMem= 2415919104 cpu: 1350.2

(Enter /home/blab/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15317 LenP2D= 41234.

LDataN: DoStor=T MaxTD1= 6 Len= 172

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

GePol: Maximum number of non-zero 1st derivatives = 253

Leave Link 701 at Tue Sep 17 14:08:28 2019, MaxMem= 2415919104 cpu: 66.6

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 14:08:28 2019, MaxMem= 2415919104 cpu: 0.3

(Enter /home/blab/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

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

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

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

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

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

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

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

Petite list used in FoFCou.

Leave Link 703 at Tue Sep 17 14:08:41 2019, MaxMem= 2415919104 cpu: 227.5

(Enter /home/blab/g09/l716.exe)

Dipole =-6.25277607D-13-9.76996262D-15 4.44089210D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000236737 0.000091318 0.000000000

2 7 0.000170261 -0.000074144 -0.000000000

3 6 0.000069821 0.000211815 0.000000000

4 6 -0.000125306 -0.000067322 -0.000000000

5 6 0.000028855 -0.000067618 0.000000000

6 7 -0.000185410 -0.000205958 0.000000000

7 6 0.000131481 0.000270578 0.000000000

8 7 -0.000052679 -0.000157276 0.000000000

9 6 0.000197770 -0.000036272 -0.000000000

10 6 -0.000039045 0.000129245 0.000000000

11 6 -0.000062544 -0.000044645 0.000000000

12 7 0.000183590 -0.000159567 -0.000000000

13 6 0.000039045 -0.000129245 0.000000000

14 6 0.000062544 0.000044645 0.000000000

15 6 -0.000131481 -0.000270578 -0.000000000

16 7 0.000052679 0.000157276 -0.000000000

17 6 -0.000197770 0.000036272 0.000000000

18 7 0.000185410 0.000205958 0.000000000

19 7 -0.000170261 0.000074144 -0.000000000

20 6 -0.000069821 -0.000211815 -0.000000000

21 6 0.000125306 0.000067322 -0.000000000

22 6 -0.000028855 0.000067618 0.000000000

23 6 0.000236737 -0.000091318 -0.000000000

24 7 -0.000183590 0.000159567 0.000000000

25 30 -0.000000000 -0.000000000 0.000000000

26 6 0.000003791 -0.000004566 -0.000000000

27 1 0.000000636 -0.000006461 0.000000000

28 6 0.000021172 0.000009595 0.000000000

29 1 0.000003556 0.000001637 0.000000000

30 6 -0.000021172 -0.000009595 -0.000000000

31 1 -0.000003556 -0.000001637 -0.000000000

32 6 -0.000003791 0.000004566 0.000000000

33 1 -0.000000636 0.000006461 0.000000000

34 1 0.000001003 0.000005369 0.000000000

35 1 0.000003212 0.000006491 0.000001065

36 1 0.000003212 0.000006491 -0.000001065

37 1 0.000001250 -0.000000709 0.000000391

38 1 0.000001250 -0.000000709 -0.000000391

39 1 0.000000665 0.000001151 0.000000000

40 1 -0.000001250 0.000000709 0.000000391

41 1 -0.000001250 0.000000709 -0.000000391

42 1 -0.000000665 -0.000001151 0.000000000

43 1 -0.000003212 -0.000006491 0.000001065

44 1 -0.000003212 -0.000006491 -0.000001065

45 1 -0.000001003 -0.000005369 0.000000000

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

Cartesian Forces: Max 0.000270578 RMS 0.000085510

Leave Link 716 at Tue Sep 17 14:08:41 2019, MaxMem= 2415919104 cpu: 0.3

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

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

Internal Forces: Max 0.000232829 RMS 0.000036695

Search for a local minimum.

Step number 11 out of a maximum of 270

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

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4 5

6 7 8 9 10

11

DE= -6.08D-07 DEPred=-1.01D-06 R= 6.01D-01

TightC=F SS= 1.41D+00 RLast= 6.51D-03 DXNew= 2.9025D-01 1.9515D-02

Trust test= 6.01D-01 RLast= 6.51D-03 DXMaxT set to 1.73D-01

ITU= 1 1 1 -1 1 1 1 0 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01329

Eigenvalues --- 0.01331 0.01340 0.01342 0.01608 0.01628

Eigenvalues --- 0.01636 0.01646 0.01771 0.01790 0.01804

Eigenvalues --- 0.01817 0.01886 0.01906 0.01937 0.01948

Eigenvalues --- 0.01997 0.01999 0.02045 0.02048 0.02070

Eigenvalues --- 0.02087 0.02102 0.02110 0.02114 0.02205

Eigenvalues --- 0.02313 0.02317 0.02352 0.02373 0.07122

Eigenvalues --- 0.07179 0.07179 0.07180 0.07180 0.07202

Eigenvalues --- 0.07288 0.07321 0.09909 0.11719 0.14496

Eigenvalues --- 0.14497 0.15243 0.15733 0.15979 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16002

Eigenvalues --- 0.16043 0.16428 0.17766 0.19959 0.21316

Eigenvalues --- 0.22072 0.22095 0.23752 0.23845 0.23861

Eigenvalues --- 0.24009 0.24633 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25010 0.25103

Eigenvalues --- 0.25550 0.27653 0.30497 0.33208 0.33209

Eigenvalues --- 0.33231 0.33260 0.33282 0.33282 0.33599

Eigenvalues --- 0.33721 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33724 0.33968 0.34387 0.34432

Eigenvalues --- 0.34437 0.34437 0.34497 0.35537 0.35548

Eigenvalues --- 0.35682 0.35682 0.35700 0.35729 0.38611

Eigenvalues --- 0.39495 0.41595 0.41774 0.41839 0.44349

Eigenvalues --- 0.47707 0.48965 0.48980 0.50586 0.51300

Eigenvalues --- 0.51360 0.51363 0.53804 0.54017 0.54023

Eigenvalues --- 0.54522 0.56330 0.56333 0.56767

DIIS coeff's: 0.75777 0.35969 -0.17762 0.05689 -0.00110

DIIS coeff's: 0.00188 0.00157 0.00092

Cosine: 0.998 > 0.500

Length: 1.045

GDIIS step was calculated using 8 of the last 8 vectors.

Iteration 1 RMS(Cart)= 0.00016656 RMS(Int)= 0.00000005

Iteration 2 RMS(Cart)= 0.00000004 RMS(Int)= 0.00000004

ITry= 1 IFail=0 DXMaxC= 7.00D-04 DCOld= 1.00D+10 DXMaxT= 1.73D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 7.63D-11 for atom 41.

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

(Linear) (Quad) (Total)

R1 2.58179 0.00013 0.00063 -0.00004 0.00059 2.58238

R2 2.71256 0.00002 0.00012 -0.00004 0.00009 2.71265

R3 2.58366 -0.00018 -0.00064 -0.00005 -0.00070 2.58296

R4 2.58412 -0.00011 -0.00052 -0.00004 -0.00056 2.58357

R5 3.80396 0.00003 0.00001 0.00002 0.00003 3.80398

R6 2.72740 0.00013 0.00056 0.00002 0.00058 2.72798

R7 2.57902 -0.00004 -0.00004 -0.00002 -0.00006 2.57896

R8 2.62429 -0.00006 -0.00026 0.00001 -0.00025 2.62404

R9 2.82502 -0.00002 -0.00009 0.00002 -0.00007 2.82495

R10 2.04554 0.00000 0.00003 -0.00002 0.00001 2.04555

R11 2.49985 0.00023 0.00074 0.00001 0.00075 2.50059

R12 2.58955 -0.00010 -0.00054 -0.00003 -0.00057 2.58898

R13 2.77754 -0.00002 -0.00013 -0.00001 -0.00014 2.77740

R14 2.58427 0.00012 0.00058 0.00003 0.00061 2.58488

R15 3.79186 0.00001 0.00017 -0.00007 0.00010 3.79196

R16 2.80324 -0.00008 -0.00053 0.00000 -0.00053 2.80271

R17 2.49711 0.00004 0.00007 -0.00005 0.00002 2.49713

R18 2.56762 0.00008 0.00029 -0.00003 0.00026 2.56788

R19 2.81597 0.00002 0.00005 0.00003 0.00008 2.81605

R20 2.04508 0.00000 -0.00001 0.00001 -0.00000 2.04508

R21 2.49711 0.00004 0.00007 -0.00005 0.00002 2.49713

R22 2.56762 0.00008 0.00029 -0.00003 0.00026 2.56788

R23 2.80324 -0.00008 -0.00053 0.00000 -0.00053 2.80271

R24 2.81597 0.00002 0.00005 0.00003 0.00008 2.81605

R25 2.77754 -0.00002 -0.00013 -0.00001 -0.00014 2.77740

R26 2.04508 0.00000 -0.00001 0.00001 -0.00000 2.04508

R27 2.58955 -0.00010 -0.00054 -0.00003 -0.00057 2.58898

R28 2.49985 0.00023 0.00074 0.00001 0.00075 2.50059

R29 2.58427 0.00012 0.00058 0.00003 0.00061 2.58488

R30 3.79186 0.00001 0.00017 -0.00007 0.00010 3.79196

R31 2.57902 -0.00004 -0.00004 -0.00002 -0.00006 2.57896

R32 2.58412 -0.00011 -0.00052 -0.00004 -0.00056 2.58357

R33 2.58179 0.00013 0.00063 -0.00004 0.00059 2.58238

R34 3.80396 0.00003 0.00001 0.00002 0.00003 3.80398

R35 2.72740 0.00013 0.00056 0.00002 0.00058 2.72798

R36 2.62429 -0.00006 -0.00026 0.00001 -0.00025 2.62404

R37 2.82502 -0.00002 -0.00009 0.00002 -0.00007 2.82495

R38 2.71256 0.00002 0.00012 -0.00004 0.00009 2.71265

R39 2.04554 0.00000 0.00003 -0.00002 0.00001 2.04555

R40 2.58366 -0.00018 -0.00064 -0.00005 -0.00070 2.58296

R41 2.06455 -0.00000 0.00000 -0.00000 -0.00000 2.06455

R42 2.07018 -0.00000 0.00001 -0.00000 0.00000 2.07019

R43 2.07018 -0.00000 0.00001 -0.00000 0.00000 2.07019

R44 2.06906 -0.00000 0.00000 -0.00001 -0.00001 2.06905

R45 2.06906 -0.00000 0.00000 -0.00001 -0.00001 2.06905

R46 2.06319 0.00000 -0.00000 0.00001 0.00000 2.06319

R47 2.06906 -0.00000 0.00000 -0.00001 -0.00001 2.06905

R48 2.06906 -0.00000 0.00000 -0.00001 -0.00001 2.06905

R49 2.06319 0.00000 -0.00000 0.00001 0.00000 2.06319

R50 2.07018 -0.00000 0.00001 -0.00000 0.00000 2.07019

R51 2.07018 -0.00000 0.00001 -0.00000 0.00000 2.07019

R52 2.06455 -0.00000 0.00000 -0.00000 -0.00000 2.06455

A1 1.88897 0.00001 -0.00009 -0.00002 -0.00010 1.88887

A2 2.20609 0.00000 -0.00005 0.00001 -0.00004 2.20605

A3 2.18812 -0.00002 0.00013 0.00001 0.00014 2.18826

A4 1.90522 -0.00002 0.00002 0.00003 0.00006 1.90528

A5 2.19259 0.00000 -0.00026 0.00004 -0.00021 2.19238

A6 2.18537 0.00001 0.00023 -0.00008 0.00016 2.18553

A7 1.89740 0.00000 -0.00001 -0.00001 -0.00002 1.89738

A8 2.21448 0.00002 0.00021 0.00003 0.00024 2.21472

A9 2.17131 -0.00002 -0.00020 -0.00001 -0.00022 2.17109

A10 1.85390 0.00002 0.00006 -0.00003 0.00004 1.85394

A11 2.18759 -0.00001 -0.00019 0.00004 -0.00014 2.18744

A12 2.24169 -0.00001 0.00012 -0.00002 0.00011 2.24180

A13 1.87928 -0.00002 0.00001 0.00002 0.00003 1.87931

A14 2.18548 0.00001 -0.00004 -0.00001 -0.00004 2.18544

A15 2.21843 0.00001 0.00003 -0.00001 0.00001 2.21844

A16 2.17823 -0.00003 -0.00042 0.00001 -0.00041 2.17782

A17 2.22887 -0.00001 0.00000 0.00003 0.00003 2.22890

A18 2.17480 0.00001 -0.00012 -0.00001 -0.00012 2.17468

A19 1.87951 -0.00000 0.00012 -0.00002 0.00009 1.87960

A20 1.91300 0.00001 -0.00003 -0.00001 -0.00004 1.91296

A21 2.18816 -0.00001 0.00025 -0.00006 0.00018 2.18834

A22 2.18203 -0.00000 -0.00022 0.00007 -0.00015 2.18189

A23 1.88644 -0.00001 -0.00005 0.00002 -0.00003 1.88641

A24 2.23926 -0.00003 -0.00028 -0.00003 -0.00030 2.23896

A25 2.15749 0.00004 0.00033 0.00000 0.00033 2.15782

A26 1.85884 -0.00002 0.00002 -0.00005 -0.00003 1.85881

A27 2.16504 0.00004 0.00021 0.00007 0.00027 2.16532

A28 2.25930 -0.00001 -0.00022 -0.00002 -0.00024 2.25906

A29 1.88700 0.00002 -0.00006 0.00006 0.00000 1.88700

A30 2.17004 -0.00001 0.00010 -0.00002 0.00008 2.17013

A31 2.22615 -0.00001 -0.00005 -0.00004 -0.00008 2.22606

A32 2.17607 0.00004 0.00053 -0.00002 0.00051 2.17657

A33 1.85884 -0.00002 0.00002 -0.00005 -0.00003 1.85881

A34 2.25930 -0.00001 -0.00022 -0.00002 -0.00024 2.25906

A35 2.16504 0.00004 0.00021 0.00007 0.00027 2.16532

A36 1.88700 0.00002 -0.00006 0.00006 0.00000 1.88700

A37 2.22615 -0.00001 -0.00005 -0.00004 -0.00008 2.22606

A38 2.17004 -0.00001 0.00010 -0.00002 0.00008 2.17013

A39 1.87951 -0.00000 0.00012 -0.00002 0.00009 1.87960

A40 2.17480 0.00001 -0.00012 -0.00001 -0.00012 2.17468

A41 2.22887 -0.00001 0.00000 0.00003 0.00003 2.22890

A42 1.91300 0.00001 -0.00003 -0.00001 -0.00004 1.91296

A43 2.18816 -0.00001 0.00025 -0.00006 0.00018 2.18834

A44 2.18203 -0.00000 -0.00022 0.00007 -0.00015 2.18189

A45 2.15749 0.00004 0.00033 0.00000 0.00033 2.15782

A46 2.23926 -0.00003 -0.00028 -0.00003 -0.00030 2.23896

A47 1.88644 -0.00001 -0.00005 0.00002 -0.00003 1.88641

A48 2.17823 -0.00003 -0.00042 0.00001 -0.00041 2.17782

A49 1.90522 -0.00002 0.00002 0.00003 0.00006 1.90528

A50 2.18537 0.00001 0.00023 -0.00008 0.00016 2.18553

A51 2.19259 0.00000 -0.00026 0.00004 -0.00021 2.19238

A52 2.21448 0.00002 0.00021 0.00003 0.00024 2.21472

A53 2.17131 -0.00002 -0.00020 -0.00001 -0.00022 2.17109

A54 1.89740 0.00000 -0.00001 -0.00001 -0.00002 1.89738

A55 1.85390 0.00002 0.00006 -0.00003 0.00004 1.85394

A56 2.18759 -0.00001 -0.00019 0.00004 -0.00014 2.18744

A57 2.24169 -0.00001 0.00012 -0.00002 0.00011 2.24180

A58 1.87928 -0.00002 0.00001 0.00002 0.00003 1.87931

A59 2.21843 0.00001 0.00003 -0.00001 0.00001 2.21844

A60 2.18548 0.00001 -0.00004 -0.00001 -0.00004 2.18544

A61 1.88897 0.00001 -0.00009 -0.00002 -0.00010 1.88887

A62 2.20609 0.00000 -0.00005 0.00001 -0.00004 2.20605

A63 2.18812 -0.00002 0.00013 0.00001 0.00014 2.18826

A64 2.17607 0.00004 0.00053 -0.00002 0.00051 2.17657

A65 1.57127 0.00001 -0.00027 0.00007 -0.00019 1.57107

A66 1.57033 -0.00001 0.00027 -0.00007 0.00019 1.57052

A67 1.57033 -0.00001 0.00027 -0.00007 0.00019 1.57052

A68 1.57127 0.00001 -0.00027 0.00007 -0.00019 1.57107

A69 1.94206 -0.00001 0.00004 -0.00005 -0.00001 1.94205

A70 1.94968 -0.00001 -0.00003 -0.00000 -0.00004 1.94964

A71 1.94968 -0.00001 -0.00003 -0.00000 -0.00004 1.94964

A72 1.88061 0.00001 0.00003 0.00001 0.00004 1.88066

A73 1.88061 0.00001 0.00003 0.00001 0.00004 1.88066

A74 1.85705 0.00001 -0.00003 0.00003 0.00001 1.85706

A75 1.93975 0.00000 0.00005 -0.00001 0.00004 1.93979

A76 1.93975 0.00000 0.00005 -0.00001 0.00004 1.93979

A77 1.94563 -0.00001 -0.00004 -0.00003 -0.00007 1.94556

A78 1.85728 0.00000 0.00001 0.00004 0.00005 1.85733

A79 1.88909 -0.00000 -0.00004 0.00001 -0.00003 1.88905

A80 1.88909 -0.00000 -0.00004 0.00001 -0.00003 1.88905

A81 1.93975 0.00000 0.00005 -0.00001 0.00004 1.93979

A82 1.93975 0.00000 0.00005 -0.00001 0.00004 1.93979

A83 1.94563 -0.00001 -0.00004 -0.00003 -0.00007 1.94556

A84 1.85728 0.00000 0.00001 0.00004 0.00005 1.85733

A85 1.88909 -0.00000 -0.00004 0.00001 -0.00003 1.88905

A86 1.88909 -0.00000 -0.00004 0.00001 -0.00003 1.88905

A87 1.94968 -0.00001 -0.00003 -0.00000 -0.00004 1.94964

A88 1.94968 -0.00001 -0.00003 -0.00000 -0.00004 1.94964

A89 1.94206 -0.00001 0.00004 -0.00005 -0.00001 1.94205

A90 1.85705 0.00001 -0.00003 0.00003 0.00001 1.85706

A91 1.88061 0.00001 0.00003 0.00001 0.00004 1.88066

A92 1.88061 0.00001 0.00003 0.00001 0.00004 1.88066

A93 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

A94 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

A95 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

A96 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D1 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D2 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D3 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D4 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D6 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D7 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D10 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D11 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D12 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D13 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D14 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D15 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D16 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D17 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D18 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D19 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D20 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D21 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D22 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D23 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D24 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D25 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D26 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D27 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D28 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D29 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D30 1.03893 0.00000 -0.00004 0.00002 -0.00002 1.03891

D31 -1.03893 -0.00000 0.00004 -0.00002 0.00002 -1.03891

D32 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.10266 0.00000 -0.00004 0.00002 -0.00002 -2.10268

D34 2.10266 -0.00000 0.00004 -0.00002 0.00002 2.10268

D35 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D36 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D37 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D38 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D39 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D40 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D41 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D42 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D43 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D44 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D45 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D46 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D47 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D48 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D49 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D50 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D51 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D52 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D53 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D54 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D55 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D56 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D57 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D58 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D59 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D60 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D61 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D62 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D63 1.03250 0.00000 0.00004 0.00002 0.00006 1.03255

D64 -1.03250 -0.00000 -0.00004 -0.00002 -0.00006 -1.03255

D65 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D66 -2.10910 0.00000 0.00004 0.00002 0.00006 -2.10904

D67 2.10910 -0.00000 -0.00004 -0.00002 -0.00006 2.10904

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D70 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D71 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D72 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D73 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D74 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D75 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D76 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D77 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D78 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D79 -2.10910 0.00000 0.00004 0.00002 0.00006 -2.10904

D80 2.10910 -0.00000 -0.00004 -0.00002 -0.00006 2.10904

D81 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D82 1.03250 0.00000 0.00004 0.00002 0.00006 1.03255

D83 -1.03250 -0.00000 -0.00004 -0.00002 -0.00006 -1.03255

D84 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D85 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D86 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D87 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D88 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D89 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D90 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D91 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D92 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D93 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D94 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D95 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D96 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D97 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D98 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D99 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D100 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D101 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D102 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D103 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D104 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D105 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D106 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D107 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D108 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D109 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D110 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D111 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D112 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D113 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D114 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D115 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D116 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D117 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D118 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D119 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D120 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D121 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D122 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D123 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D124 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D125 1.03893 0.00000 -0.00004 0.00002 -0.00002 1.03891

D126 -1.03893 -0.00000 0.00004 -0.00002 0.00002 -1.03891

D127 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D128 -2.10266 0.00000 -0.00004 0.00002 -0.00002 -2.10268

D129 2.10266 -0.00000 0.00004 -0.00002 0.00002 2.10268

D130 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D131 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D132 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D133 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D134 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D135 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D136 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

Item Value Threshold Converged?

Maximum Force 0.000233 0.000450 YES

RMS Force 0.000037 0.000300 YES

Maximum Displacement 0.000700 0.001800 YES

RMS Displacement 0.000167 0.001200 YES

Predicted change in Energy=-7.645047D-07

Optimization completed.

-- Stationary point found.

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! Optimized Parameters !

! (Angstroms and Degrees) !

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! Name Definition Value Derivative Info. !

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! R1 R(1,2) 1.3662 -DE/DX = 0.0001 !

! R2 R(1,5) 1.4354 -DE/DX = 0.0 !

! R3 R(1,12) 1.3672 -DE/DX = -0.0002 !

! R4 R(2,3) 1.3675 -DE/DX = -0.0001 !

! R5 R(2,25) 2.013 -DE/DX = 0.0 !

! R6 R(3,4) 1.4433 -DE/DX = 0.0001 !

! R7 R(3,6) 1.3648 -DE/DX = 0.0 !

! R8 R(4,5) 1.3887 -DE/DX = -0.0001 !

! R9 R(4,26) 1.4949 -DE/DX = 0.0 !

! R10 R(5,27) 1.0825 -DE/DX = 0.0 !

! R11 R(6,7) 1.3229 -DE/DX = 0.0002 !

! R12 R(7,8) 1.3703 -DE/DX = -0.0001 !

! R13 R(7,11) 1.4698 -DE/DX = 0.0 !

! R14 R(8,9) 1.3675 -DE/DX = 0.0001 !

! R15 R(8,25) 2.0066 -DE/DX = 0.0 !

! R16 R(9,10) 1.4834 -DE/DX = -0.0001 !

! R17 R(9,24) 1.3214 -DE/DX = 0.0 !

! R18 R(10,11) 1.3587 -DE/DX = 0.0001 !

! R19 R(10,28) 1.4901 -DE/DX = 0.0 !

! R20 R(11,29) 1.0822 -DE/DX = 0.0 !

! R21 R(12,17) 1.3214 -DE/DX = 0.0 !

! R22 R(13,14) 1.3587 -DE/DX = 0.0001 !

! R23 R(13,17) 1.4834 -DE/DX = -0.0001 !

! R24 R(13,30) 1.4901 -DE/DX = 0.0 !

! R25 R(14,15) 1.4698 -DE/DX = 0.0 !

! R26 R(14,31) 1.0822 -DE/DX = 0.0 !

! R27 R(15,16) 1.3703 -DE/DX = -0.0001 !

! R28 R(15,18) 1.3229 -DE/DX = 0.0002 !

! R29 R(16,17) 1.3675 -DE/DX = 0.0001 !

! R30 R(16,25) 2.0066 -DE/DX = 0.0 !

! R31 R(18,20) 1.3648 -DE/DX = 0.0 !

! R32 R(19,20) 1.3675 -DE/DX = -0.0001 !

! R33 R(19,23) 1.3662 -DE/DX = 0.0001 !

! R34 R(19,25) 2.013 -DE/DX = 0.0 !

! R35 R(20,21) 1.4433 -DE/DX = 0.0001 !

! R36 R(21,22) 1.3887 -DE/DX = -0.0001 !

! R37 R(21,32) 1.4949 -DE/DX = 0.0 !

! R38 R(22,23) 1.4354 -DE/DX = 0.0 !

! R39 R(22,33) 1.0825 -DE/DX = 0.0 !

! R40 R(23,24) 1.3672 -DE/DX = -0.0002 !

! R41 R(26,34) 1.0925 -DE/DX = 0.0 !

! R42 R(26,35) 1.0955 -DE/DX = 0.0 !

! R43 R(26,36) 1.0955 -DE/DX = 0.0 !

! R44 R(28,37) 1.0949 -DE/DX = 0.0 !

! R45 R(28,38) 1.0949 -DE/DX = 0.0 !

! R46 R(28,39) 1.0918 -DE/DX = 0.0 !

! R47 R(30,40) 1.0949 -DE/DX = 0.0 !

! R48 R(30,41) 1.0949 -DE/DX = 0.0 !

! R49 R(30,42) 1.0918 -DE/DX = 0.0 !

! R50 R(32,43) 1.0955 -DE/DX = 0.0 !

! R51 R(32,44) 1.0955 -DE/DX = 0.0 !

! R52 R(32,45) 1.0925 -DE/DX = 0.0 !

! A1 A(2,1,5) 108.2301 -DE/DX = 0.0 !

! A2 A(2,1,12) 126.3997 -DE/DX = 0.0 !

! A3 A(5,1,12) 125.3703 -DE/DX = 0.0 !

! A4 A(1,2,3) 109.1613 -DE/DX = 0.0 !

! A5 A(1,2,25) 125.6263 -DE/DX = 0.0 !

! A6 A(3,2,25) 125.2124 -DE/DX = 0.0 !

! A7 A(2,3,4) 108.7131 -DE/DX = 0.0 !

! A8 A(2,3,6) 126.8802 -DE/DX = 0.0 !

! A9 A(4,3,6) 124.4067 -DE/DX = 0.0 !

! A10 A(3,4,5) 106.2209 -DE/DX = 0.0 !

! A11 A(3,4,26) 125.3396 -DE/DX = 0.0 !

! A12 A(5,4,26) 128.4395 -DE/DX = 0.0 !

! A13 A(1,5,4) 107.6746 -DE/DX = 0.0 !

! A14 A(1,5,27) 125.2188 -DE/DX = 0.0 !

! A15 A(4,5,27) 127.1066 -DE/DX = 0.0 !

! A16 A(3,6,7) 124.8033 -DE/DX = 0.0 !

! A17 A(6,7,8) 127.705 -DE/DX = 0.0 !

! A18 A(6,7,11) 124.6071 -DE/DX = 0.0 !

! A19 A(8,7,11) 107.6879 -DE/DX = 0.0 !

! A20 A(7,8,9) 109.6065 -DE/DX = 0.0 !

! A21 A(7,8,25) 125.3721 -DE/DX = 0.0 !

! A22 A(9,8,25) 125.0213 -DE/DX = 0.0 !

! A23 A(8,9,10) 108.0848 -DE/DX = 0.0 !

! A24 A(8,9,24) 128.3002 -DE/DX = 0.0 !

! A25 A(10,9,24) 123.615 -DE/DX = 0.0 !

! A26 A(9,10,11) 106.5039 -DE/DX = 0.0 !

! A27 A(9,10,28) 124.0479 -DE/DX = 0.0 !

! A28 A(11,10,28) 129.4483 -DE/DX = 0.0 !

! A29 A(7,11,10) 108.1169 -DE/DX = 0.0 !

! A30 A(7,11,29) 124.3342 -DE/DX = 0.0 !

! A31 A(10,11,29) 127.5489 -DE/DX = 0.0 !

! A32 A(1,12,17) 124.6795 -DE/DX = 0.0 !

! A33 A(14,13,17) 106.5039 -DE/DX = 0.0 !

! A34 A(14,13,30) 129.4483 -DE/DX = 0.0 !

! A35 A(17,13,30) 124.0479 -DE/DX = 0.0 !

! A36 A(13,14,15) 108.1169 -DE/DX = 0.0 !

! A37 A(13,14,31) 127.5489 -DE/DX = 0.0 !

! A38 A(15,14,31) 124.3342 -DE/DX = 0.0 !

! A39 A(14,15,16) 107.6879 -DE/DX = 0.0 !

! A40 A(14,15,18) 124.6071 -DE/DX = 0.0 !

! A41 A(16,15,18) 127.705 -DE/DX = 0.0 !

! A42 A(15,16,17) 109.6065 -DE/DX = 0.0 !

! A43 A(15,16,25) 125.3721 -DE/DX = 0.0 !

! A44 A(17,16,25) 125.0213 -DE/DX = 0.0 !

! A45 A(12,17,13) 123.615 -DE/DX = 0.0 !

! A46 A(12,17,16) 128.3002 -DE/DX = 0.0 !

! A47 A(13,17,16) 108.0848 -DE/DX = 0.0 !

! A48 A(15,18,20) 124.8033 -DE/DX = 0.0 !

! A49 A(20,19,23) 109.1613 -DE/DX = 0.0 !

! A50 A(20,19,25) 125.2124 -DE/DX = 0.0 !

! A51 A(23,19,25) 125.6263 -DE/DX = 0.0 !

! A52 A(18,20,19) 126.8802 -DE/DX = 0.0 !

! A53 A(18,20,21) 124.4067 -DE/DX = 0.0 !

! A54 A(19,20,21) 108.7131 -DE/DX = 0.0 !

! A55 A(20,21,22) 106.2209 -DE/DX = 0.0 !

! A56 A(20,21,32) 125.3396 -DE/DX = 0.0 !

! A57 A(22,21,32) 128.4395 -DE/DX = 0.0 !

! A58 A(21,22,23) 107.6746 -DE/DX = 0.0 !

! A59 A(21,22,33) 127.1066 -DE/DX = 0.0 !

! A60 A(23,22,33) 125.2188 -DE/DX = 0.0 !

! A61 A(19,23,22) 108.2301 -DE/DX = 0.0 !

! A62 A(19,23,24) 126.3997 -DE/DX = 0.0 !

! A63 A(22,23,24) 125.3703 -DE/DX = 0.0 !

! A64 A(9,24,23) 124.6795 -DE/DX = 0.0 !

! A65 A(2,25,8) 90.027 -DE/DX = 0.0 !

! A66 A(2,25,16) 89.973 -DE/DX = 0.0 !

! A67 A(8,25,19) 89.973 -DE/DX = 0.0 !

! A68 A(16,25,19) 90.027 -DE/DX = 0.0 !

! A69 A(4,26,34) 111.272 -DE/DX = 0.0 !

! A70 A(4,26,35) 111.7082 -DE/DX = 0.0 !

! A71 A(4,26,36) 111.7082 -DE/DX = 0.0 !

! A72 A(34,26,35) 107.7511 -DE/DX = 0.0 !

! A73 A(34,26,36) 107.7511 -DE/DX = 0.0 !

! A74 A(35,26,36) 106.4014 -DE/DX = 0.0 !

! A75 A(10,28,37) 111.1392 -DE/DX = 0.0 !

! A76 A(10,28,38) 111.1392 -DE/DX = 0.0 !

! A77 A(10,28,39) 111.4764 -DE/DX = 0.0 !

! A78 A(37,28,38) 106.4141 -DE/DX = 0.0 !

! A79 A(37,28,39) 108.2366 -DE/DX = 0.0 !

! A80 A(38,28,39) 108.2366 -DE/DX = 0.0 !

! A81 A(13,30,40) 111.1392 -DE/DX = 0.0 !

! A82 A(13,30,41) 111.1392 -DE/DX = 0.0 !

! A83 A(13,30,42) 111.4764 -DE/DX = 0.0 !

! A84 A(40,30,41) 106.4141 -DE/DX = 0.0 !

! A85 A(40,30,42) 108.2366 -DE/DX = 0.0 !

! A86 A(41,30,42) 108.2366 -DE/DX = 0.0 !

! A87 A(21,32,43) 111.7082 -DE/DX = 0.0 !

! A88 A(21,32,44) 111.7082 -DE/DX = 0.0 !

! A89 A(21,32,45) 111.272 -DE/DX = 0.0 !

! A90 A(43,32,44) 106.4014 -DE/DX = 0.0 !

! A91 A(43,32,45) 107.7511 -DE/DX = 0.0 !

! A92 A(44,32,45) 107.7511 -DE/DX = 0.0 !

! A93 L(2,25,19,16,-1) 180.0 -DE/DX = 0.0 !

! A94 L(8,25,16,19,-1) 180.0 -DE/DX = 0.0 !

! A95 L(2,25,19,16,-2) 180.0 -DE/DX = 0.0 !

! A96 L(8,25,16,19,-2) 180.0 -DE/DX = 0.0 !

! D1 D(5,1,2,3) 0.0 -DE/DX = 0.0 !

! D2 D(5,1,2,25) 180.0 -DE/DX = 0.0 !

! D3 D(12,1,2,3) 180.0 -DE/DX = 0.0 !

! D4 D(12,1,2,25) 0.0 -DE/DX = 0.0 !

! D5 D(2,1,5,4) 0.0 -DE/DX = 0.0 !

! D6 D(2,1,5,27) 180.0 -DE/DX = 0.0 !

! D7 D(12,1,5,4) 180.0 -DE/DX = 0.0 !

! D8 D(12,1,5,27) 0.0 -DE/DX = 0.0 !

! D9 D(2,1,12,17) 0.0 -DE/DX = 0.0 !

! D10 D(5,1,12,17) 180.0 -DE/DX = 0.0 !

! D11 D(1,2,3,4) 0.0 -DE/DX = 0.0 !

! D12 D(1,2,3,6) 180.0 -DE/DX = 0.0 !

! D13 D(25,2,3,4) 180.0 -DE/DX = 0.0 !

! D14 D(25,2,3,6) 0.0 -DE/DX = 0.0 !

! D15 D(1,2,25,8) 180.0 -DE/DX = 0.0 !

! D16 D(1,2,25,16) 0.0 -DE/DX = 0.0 !

! D17 D(3,2,25,8) 0.0 -DE/DX = 0.0 !

! D18 D(3,2,25,16) 180.0 -DE/DX = 0.0 !

! D19 D(2,3,4,5) 0.0 -DE/DX = 0.0 !

! D20 D(2,3,4,26) 180.0 -DE/DX = 0.0 !

! D21 D(6,3,4,5) 180.0 -DE/DX = 0.0 !

! D22 D(6,3,4,26) 0.0 -DE/DX = 0.0 !

! D23 D(2,3,6,7) 0.0 -DE/DX = 0.0 !

! D24 D(4,3,6,7) 180.0 -DE/DX = 0.0 !

! D25 D(3,4,5,1) 0.0 -DE/DX = 0.0 !

! D26 D(3,4,5,27) 180.0 -DE/DX = 0.0 !

! D27 D(26,4,5,1) 180.0 -DE/DX = 0.0 !

! D28 D(26,4,5,27) 0.0 -DE/DX = 0.0 !

! D29 D(3,4,26,34) 180.0 -DE/DX = 0.0 !

! D30 D(3,4,26,35) 59.5263 -DE/DX = 0.0 !

! D31 D(3,4,26,36) -59.5263 -DE/DX = 0.0 !

! D32 D(5,4,26,34) 0.0 -DE/DX = 0.0 !

! D33 D(5,4,26,35) -120.4737 -DE/DX = 0.0 !

! D34 D(5,4,26,36) 120.4737 -DE/DX = 0.0 !

! D35 D(3,6,7,8) 0.0 -DE/DX = 0.0 !

! D36 D(3,6,7,11) 180.0 -DE/DX = 0.0 !

! D37 D(6,7,8,9) 180.0 -DE/DX = 0.0 !

! D38 D(6,7,8,25) 0.0 -DE/DX = 0.0 !

! D39 D(11,7,8,9) 0.0 -DE/DX = 0.0 !

! D40 D(11,7,8,25) 180.0 -DE/DX = 0.0 !

! D41 D(6,7,11,10) 180.0 -DE/DX = 0.0 !

! D42 D(6,7,11,29) 0.0 -DE/DX = 0.0 !

! D43 D(8,7,11,10) 0.0 -DE/DX = 0.0 !

! D44 D(8,7,11,29) 180.0 -DE/DX = 0.0 !

! D45 D(7,8,9,10) 0.0 -DE/DX = 0.0 !

! D46 D(7,8,9,24) 180.0 -DE/DX = 0.0 !

! D47 D(25,8,9,10) 180.0 -DE/DX = 0.0 !

! D48 D(25,8,9,24) 0.0 -DE/DX = 0.0 !

! D49 D(7,8,25,2) 0.0 -DE/DX = 0.0 !

! D50 D(7,8,25,19) 180.0 -DE/DX = 0.0 !

! D51 D(9,8,25,2) 180.0 -DE/DX = 0.0 !

! D52 D(9,8,25,19) 0.0 -DE/DX = 0.0 !

! D53 D(8,9,10,11) 0.0 -DE/DX = 0.0 !

! D54 D(8,9,10,28) 180.0 -DE/DX = 0.0 !

! D55 D(24,9,10,11) 180.0 -DE/DX = 0.0 !

! D56 D(24,9,10,28) 0.0 -DE/DX = 0.0 !

! D57 D(8,9,24,23) 0.0 -DE/DX = 0.0 !

! D58 D(10,9,24,23) 180.0 -DE/DX = 0.0 !

! D59 D(9,10,11,7) 0.0 -DE/DX = 0.0 !

! D60 D(9,10,11,29) 180.0 -DE/DX = 0.0 !

! D61 D(28,10,11,7) 180.0 -DE/DX = 0.0 !

! D62 D(28,10,11,29) 0.0 -DE/DX = 0.0 !

! D63 D(9,10,28,37) 59.1577 -DE/DX = 0.0 !

! D64 D(9,10,28,38) -59.1577 -DE/DX = 0.0 !

! D65 D(9,10,28,39) 180.0 -DE/DX = 0.0 !

! D66 D(11,10,28,37) -120.8423 -DE/DX = 0.0 !

! D67 D(11,10,28,38) 120.8423 -DE/DX = 0.0 !

! D68 D(11,10,28,39) 0.0 -DE/DX = 0.0 !

! D69 D(1,12,17,13) 180.0 -DE/DX = 0.0 !

! D70 D(1,12,17,16) 0.0 -DE/DX = 0.0 !

! D71 D(17,13,14,15) 0.0 -DE/DX = 0.0 !

! D72 D(17,13,14,31) 180.0 -DE/DX = 0.0 !

! D73 D(30,13,14,15) 180.0 -DE/DX = 0.0 !

! D74 D(30,13,14,31) 0.0 -DE/DX = 0.0 !

! D75 D(14,13,17,12) 180.0 -DE/DX = 0.0 !

! D76 D(14,13,17,16) 0.0 -DE/DX = 0.0 !

! D77 D(30,13,17,12) 0.0 -DE/DX = 0.0 !

! D78 D(30,13,17,16) 180.0 -DE/DX = 0.0 !

! D79 D(14,13,30,40) -120.8423 -DE/DX = 0.0 !

! D80 D(14,13,30,41) 120.8423 -DE/DX = 0.0 !

! D81 D(14,13,30,42) 0.0 -DE/DX = 0.0 !

! D82 D(17,13,30,40) 59.1577 -DE/DX = 0.0 !

! D83 D(17,13,30,41) -59.1577 -DE/DX = 0.0 !

! D84 D(17,13,30,42) 180.0 -DE/DX = 0.0 !

! D85 D(13,14,15,16) 0.0 -DE/DX = 0.0 !

! D86 D(13,14,15,18) 180.0 -DE/DX = 0.0 !

! D87 D(31,14,15,16) 180.0 -DE/DX = 0.0 !

! D88 D(31,14,15,18) 0.0 -DE/DX = 0.0 !

! D89 D(14,15,16,17) 0.0 -DE/DX = 0.0 !

! D90 D(14,15,16,25) 180.0 -DE/DX = 0.0 !

! D91 D(18,15,16,17) 180.0 -DE/DX = 0.0 !

! D92 D(18,15,16,25) 0.0 -DE/DX = 0.0 !

! D93 D(14,15,18,20) 180.0 -DE/DX = 0.0 !

! D94 D(16,15,18,20) 0.0 -DE/DX = 0.0 !

! D95 D(15,16,17,12) 180.0 -DE/DX = 0.0 !

! D96 D(15,16,17,13) 0.0 -DE/DX = 0.0 !

! D97 D(25,16,17,12) 0.0 -DE/DX = 0.0 !

! D98 D(25,16,17,13) 180.0 -DE/DX = 0.0 !

! D99 D(15,16,25,2) 180.0 -DE/DX = 0.0 !

! D100 D(15,16,25,19) 0.0 -DE/DX = 0.0 !

! D101 D(17,16,25,2) 0.0 -DE/DX = 0.0 !

! D102 D(17,16,25,19) 180.0 -DE/DX = 0.0 !

! D103 D(15,18,20,19) 0.0 -DE/DX = 0.0 !

! D104 D(15,18,20,21) 180.0 -DE/DX = 0.0 !

! D105 D(23,19,20,18) 180.0 -DE/DX = 0.0 !

! D106 D(23,19,20,21) 0.0 -DE/DX = 0.0 !

! D107 D(25,19,20,18) 0.0 -DE/DX = 0.0 !

! D108 D(25,19,20,21) 180.0 -DE/DX = 0.0 !

! D109 D(20,19,23,22) 0.0 -DE/DX = 0.0 !

! D110 D(20,19,23,24) 180.0 -DE/DX = 0.0 !

! D111 D(25,19,23,22) 180.0 -DE/DX = 0.0 !

! D112 D(25,19,23,24) 0.0 -DE/DX = 0.0 !

! D113 D(20,19,25,8) 180.0 -DE/DX = 0.0 !

! D114 D(20,19,25,16) 0.0 -DE/DX = 0.0 !

! D115 D(23,19,25,8) 0.0 -DE/DX = 0.0 !

! D116 D(23,19,25,16) 180.0 -DE/DX = 0.0 !

! D117 D(18,20,21,22) 180.0 -DE/DX = 0.0 !

! D118 D(18,20,21,32) 0.0 -DE/DX = 0.0 !

! D119 D(19,20,21,22) 0.0 -DE/DX = 0.0 !

! D120 D(19,20,21,32) 180.0 -DE/DX = 0.0 !

! D121 D(20,21,22,23) 0.0 -DE/DX = 0.0 !

! D122 D(20,21,22,33) 180.0 -DE/DX = 0.0 !

! D123 D(32,21,22,23) 180.0 -DE/DX = 0.0 !

! D124 D(32,21,22,33) 0.0 -DE/DX = 0.0 !

! D125 D(20,21,32,43) 59.5263 -DE/DX = 0.0 !

! D126 D(20,21,32,44) -59.5263 -DE/DX = 0.0 !

! D127 D(20,21,32,45) 180.0 -DE/DX = 0.0 !

! D128 D(22,21,32,43) -120.4737 -DE/DX = 0.0 !

! D129 D(22,21,32,44) 120.4737 -DE/DX = 0.0 !

! D130 D(22,21,32,45) 0.0 -DE/DX = 0.0 !

! D131 D(21,22,23,19) 0.0 -DE/DX = 0.0 !

! D132 D(21,22,23,24) 180.0 -DE/DX = 0.0 !

! D133 D(33,22,23,19) 180.0 -DE/DX = 0.0 !

! D134 D(33,22,23,24) 0.0 -DE/DX = 0.0 !

! D135 D(19,23,24,9) 0.0 -DE/DX = 0.0 !

! D136 D(22,23,24,9) 180.0 -DE/DX = 0.0 !

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Largest change from initial coordinates is atom 39 3.406 Angstoms.

Leave Link 103 at Tue Sep 17 14:08:41 2019, MaxMem= 2415919104 cpu: 1.6

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

Input orientation:

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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1 6 0 -2.074998 -2.194745 -0.000000

2 7 0 -0.748240 -1.868735 -0.000000

3 6 0 -0.004140 -3.016019 -0.000000

4 6 0 -0.899058 -4.148349 -0.000000

5 6 0 -2.185745 -3.625892 -0.000000

6 7 0 1.357438 -3.109171 -0.000000

7 6 0 2.184855 -2.077015 -0.000000

8 7 0 1.863145 -0.744985 -0.000000

9 6 0 3.007653 0.003518 -0.000000

10 6 0 4.164855 -0.924592 -0.000000

11 6 0 3.650885 -2.182357 -0.000000

12 7 0 -3.125480 -1.319668 -0.000000

13 6 0 -4.164855 0.924592 -0.000000

14 6 0 -3.650885 2.182357 -0.000000

15 6 0 -2.184855 2.077015 -0.000000

16 7 0 -1.863145 0.744985 -0.000000

17 6 0 -3.007653 -0.003518 -0.000000

18 7 0 -1.357438 3.109171 -0.000000

19 7 0 0.748240 1.868735 -0.000000

20 6 0 0.004140 3.016019 -0.000000

21 6 0 0.899058 4.148349 -0.000000

22 6 0 2.185745 3.625892 -0.000000

23 6 0 2.074998 2.194745 -0.000000

24 7 0 3.125480 1.319668 -0.000000

25 30 0 0.000000 -0.000000 -0.000000

26 6 0 -0.478478 -5.582904 -0.000000

27 1 0 -3.115587 -4.180055 -0.000000

28 6 0 5.588193 -0.483411 -0.000000

29 1 0 4.195655 -3.117454 -0.000000

30 6 0 -5.588193 0.483411 -0.000000

31 1 0 -4.195655 3.117454 -0.000000

32 6 0 0.478478 5.582904 -0.000000

33 1 0 3.115587 4.180055 -0.000000

34 1 0 -1.343927 -6.249676 -0.000000

35 1 0 0.130841 -5.826522 0.877204

36 1 0 0.130841 -5.826522 -0.877204

37 1 0 5.810342 0.133576 0.876799

38 1 0 5.810342 0.133576 -0.876799

39 1 0 6.270796 -1.335504 -0.000000

40 1 0 -5.810342 -0.133576 0.876799

41 1 0 -5.810342 -0.133576 -0.876799

42 1 0 -6.270796 1.335504 -0.000000

43 1 0 -0.130841 5.826522 0.877204

44 1 0 -0.130841 5.826522 -0.877204

45 1 0 1.343927 6.249676 -0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.366225 0.000000

3 C 2.227767 1.367459 0.000000

4 C 2.280220 2.284598 1.443278 0.000000

5 C 1.435425 2.270247 2.265247 1.388714 0.000000

6 N 3.552153 2.443883 1.364761 2.484284 3.580663

7 C 4.261480 2.940481 2.381896 3.714962 4.636934

8 N 4.196520 2.842912 2.940128 4.383224 4.969219

9 C 5.537663 4.196673 4.264798 5.700912 6.335929

10 C 6.367814 5.002990 4.664181 6.002984 6.901242

11 C 5.725896 4.410290 3.748893 4.956521 6.012490

12 N 1.367213 2.439824 3.552516 3.599777 2.490336

13 C 3.754699 4.413155 5.730616 6.033255 4.962236

14 C 4.652143 4.983642 6.349949 6.902926 5.990191

15 C 4.273173 4.199144 5.540263 6.356763 5.702908

16 N 2.947354 2.841574 4.195360 4.987402 4.382766

17 C 2.381453 2.929843 4.253969 4.650355 3.714448

18 N 5.352235 5.015044 6.272907 7.271981 6.785806

19 N 4.947984 4.025933 4.942357 6.238501 6.228900

20 C 5.610247 4.942357 6.032043 7.221076 6.993610

21 C 7.005702 6.238501 7.221076 8.489312 8.363901

22 C 7.213442 6.228900 6.993610 8.363901 8.467484

23 C 6.040703 4.947984 5.610247 7.005702 7.213442

24 N 6.276628 5.017132 5.347214 6.789411 7.257249

25 Zn 3.020352 2.012966 3.016022 4.244656 4.233742

26 C 3.745464 3.723953 2.610344 1.494936 2.597047

27 H 2.241491 3.308555 3.322060 2.216756 1.082453

28 C 7.851953 6.486101 6.139079 7.450919 8.385064

29 H 6.338177 5.099157 4.201020 5.197965 6.401623

30 C 4.417585 5.381239 6.589966 6.590994 5.335075

31 H 5.719847 6.061910 7.428882 7.978687 7.036509

32 C 8.186090 7.551938 8.612456 9.828270 9.586449

33 H 8.220721 7.177536 7.843225 9.245523 9.435939

34 H 4.120307 4.421254 3.500224 2.147902 2.755522

35 H 4.338781 4.148054 2.947310 2.155561 3.313432

36 H 4.338781 4.148054 2.947310 2.155561 3.313432

37 H 8.268521 6.913250 6.670601 8.007478 8.879177

38 H 8.268521 6.913250 6.670601 8.007478 8.879177

39 H 8.389910 7.039262 6.496073 7.701877 8.761219

40 H 4.355455 5.422585 6.541348 6.403741 5.109085

41 H 4.355455 5.422585 6.541348 6.403741 5.109085

42 H 5.483373 6.384808 7.629334 7.676472 6.426749

43 H 8.299998 7.769663 8.886848 10.042794 9.712891

44 H 8.299998 7.769663 8.886848 10.042794 9.712891

45 H 9.110285 8.383660 9.363246 10.637195 10.487394

6 7 8 9 10

6 N 0.000000

7 C 1.322862 0.000000

8 N 2.417668 1.370330 0.000000

9 C 3.523073 2.237324 1.367536 0.000000

10 C 3.557242 2.290956 2.308707 1.483410 0.000000

11 C 2.473637 1.469810 2.293916 2.278551 1.358726

12 N 4.826891 5.364068 5.021617 6.274244 7.301031

13 C 6.838638 7.023423 6.254940 7.231407 8.532500

14 C 7.285847 7.224826 6.242904 7.005959 8.410643

15 C 6.280475 6.029124 4.934571 5.591201 7.023423

16 N 5.022616 4.934571 4.013134 4.926910 6.254940

17 C 5.357154 5.591201 4.926910 6.015310 7.231407

18 N 6.785155 6.280475 5.022616 5.357154 6.838638

19 N 5.015044 4.199144 2.841574 2.929843 4.413155

20 C 6.272907 5.540263 4.195360 4.253969 5.730616

21 C 7.271981 6.356763 4.987402 4.650355 6.033255

22 C 6.785806 5.702908 4.382766 3.714448 4.962236

23 C 5.352235 4.273173 2.947354 2.381453 3.754699

24 N 4.768708 3.524518 2.419975 1.321413 2.473258

25 Zn 3.392577 3.014562 2.006567 3.007655 4.266250

26 C 3.080575 4.402794 5.374818 6.584924 6.577265

27 H 4.599429 5.702409 6.048759 7.415953 7.975141

28 C 4.979347 3.757963 3.734220 2.626078 1.490145

29 H 2.838229 2.264029 3.327043 3.339434 2.193078

30 C 7.819747 8.183890 7.551913 8.609231 9.854157

31 H 8.343123 8.227601 7.185227 7.847563 9.286348

32 C 8.736403 7.847680 6.477614 6.125869 7.479096

33 H 7.498260 6.325915 5.081794 4.177931 5.211371

34 H 4.142480 5.464741 6.370788 7.618313 7.661801

35 H 3.107737 4.364317 5.439889 6.560100 6.408718

36 H 3.107737 4.364317 5.439889 6.560100 6.408718

37 H 5.577861 4.335856 4.137754 2.939516 2.143857

38 H 5.577861 4.335856 4.137754 2.939516 2.143857

39 H 5.223695 4.152681 4.447033 3.527192 2.145656

40 H 7.810251 8.274594 7.747580 8.862539 10.044851

41 H 7.810251 8.274594 7.747580 8.862539 10.044851

42 H 8.828652 9.118297 8.395799 9.373570 10.677587

43 H 9.101158 8.282382 6.923162 6.672856 8.049847

44 H 9.101158 8.282382 6.923162 6.672856 8.049847

45 H 9.358857 8.369047 7.013905 6.463936 7.708941

11 12 13 14 15

11 C 0.000000

12 N 6.831057 0.000000

13 C 8.410643 2.473258 0.000000

14 C 8.506854 3.541218 1.358726 0.000000

15 C 7.224826 3.524518 2.290956 1.469810 0.000000

16 N 6.242904 2.419975 2.308707 2.293916 1.370330

17 C 7.005959 1.321413 1.483410 2.278551 2.237324

18 N 7.285847 4.768708 3.557242 2.473637 1.322862

19 N 4.983642 5.017132 5.002990 4.410290 2.940481

20 C 6.349949 5.347214 4.664181 3.748893 2.381896

21 C 6.902926 6.789411 6.002984 4.956521 3.714962

22 C 5.990191 7.257249 6.901242 6.012490 4.636934

23 C 4.652143 6.276628 6.367814 5.725896 4.261480

24 N 3.541218 6.785321 7.301031 6.831057 5.364068

25 Zn 4.253427 3.392660 4.266250 4.253427 3.014562

26 C 5.349333 5.018147 7.479096 8.388292 7.847680

27 H 7.055207 2.860405 5.211371 6.384891 6.325915

28 C 2.576738 8.753708 9.854157 9.615970 8.183890

29 H 1.082212 7.538637 9.286348 9.468695 8.227601

30 C 9.615970 3.052221 1.490145 2.576738 3.757963

31 H 9.468695 4.564354 2.193078 1.082212 2.264029

32 C 8.388292 7.786784 6.577265 5.349333 4.402794

33 H 6.384891 8.318526 7.975141 7.055207 5.702409

34 H 6.441369 5.242034 7.708941 8.741924 8.369047

35 H 5.141998 5.628930 8.049847 8.900173 8.282382

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37 H 3.285662 9.095581 10.044851 9.720138 8.274594

38 H 3.285662 9.095581 10.044851 9.720138 8.274594

39 H 2.753379 9.396289 10.677587 10.526875 9.118297

40 H 9.720138 3.063344 2.143857 3.285662 4.335856

41 H 9.720138 3.063344 2.143857 3.285662 4.335856

42 H 10.526875 4.116182 2.145656 2.753379 4.152681

43 H 8.900173 7.797780 6.408718 5.141998 4.364317

44 H 8.900173 7.797780 6.408718 5.141998 4.364317

45 H 8.741924 8.790367 7.661801 6.441369 5.464741

16 17 18 19 20

16 N 0.000000

17 C 1.367536 0.000000

18 N 2.417668 3.523073 0.000000

19 N 2.842912 4.196673 2.443883 0.000000

20 C 2.940128 4.264798 1.364761 1.367459 0.000000

21 C 4.383224 5.700912 2.484284 2.284598 1.443278

22 C 4.969219 6.335929 3.580663 2.270247 2.265247

23 C 4.196520 5.537663 3.552153 1.366225 2.227767

24 N 5.021617 6.274244 4.826891 2.439824 3.552516

25 Zn 2.006567 3.007655 3.392577 2.012966 3.016022

26 C 6.477614 6.125869 8.736403 7.551938 8.612456

27 H 5.081794 4.177931 7.498260 7.177536 7.843225

28 C 7.551913 8.609231 7.819747 5.381239 6.589966

29 H 7.185227 7.847563 8.343123 6.061910 7.428882

30 C 3.734220 2.626078 4.979347 6.486101 6.139079

31 H 3.327043 3.339434 2.838229 5.099157 4.201020

32 C 5.374818 6.584924 3.080575 3.723953 2.610344

33 H 6.048759 7.415953 4.599429 3.308555 3.322060

34 H 7.013905 6.463936 9.358857 8.383660 9.363246

35 H 6.923162 6.672856 9.101158 7.769663 8.886848

36 H 6.923162 6.672856 9.101158 7.769663 8.886848

37 H 7.747580 8.862539 7.810251 5.422585 6.541348

38 H 7.747580 8.862539 7.810251 5.422585 6.541348

39 H 8.395799 9.373570 8.828652 6.384808 7.629334

40 H 4.137754 2.939516 5.577861 6.913250 6.670601

41 H 4.137754 2.939516 5.577861 6.913250 6.670601

42 H 4.447033 3.527192 5.223695 7.039262 6.496073

43 H 5.439889 6.560100 3.107737 4.148054 2.947310

44 H 5.439889 6.560100 3.107737 4.148054 2.947310

45 H 6.370788 7.618313 4.142480 4.421254 3.500224

21 22 23 24 25

21 C 0.000000

22 C 1.388714 0.000000

23 C 2.280220 1.435425 0.000000

24 N 3.599777 2.490336 1.367213 0.000000

25 Zn 4.244656 4.233742 3.020352 3.392660 0.000000

26 C 9.828270 9.586449 8.186090 7.786784 5.603370

27 H 9.245523 9.435939 8.220721 8.318526 5.213420

28 C 6.590994 5.335075 4.417585 3.052221 5.609063

29 H 7.978687 7.036509 5.719847 4.564354 5.227049

30 C 7.450919 8.385064 7.851953 8.753708 5.609063

31 H 5.197965 6.401623 6.338177 7.538637 5.227049

32 C 1.494936 2.597047 3.745464 5.018147 5.603370

33 H 2.216756 1.082453 2.241491 2.860405 5.213420

34 H 10.637195 10.487394 9.110285 8.790367 6.392542

35 H 10.042794 9.712891 8.299998 7.797780 5.893638

36 H 10.042794 9.712891 8.299998 7.797780 5.893638

37 H 6.403741 5.109085 4.355455 3.063344 5.877643

38 H 6.403741 5.109085 4.355455 3.063344 5.877643

39 H 7.676472 6.426749 5.483373 4.116182 6.411432

40 H 8.007478 8.879177 8.268521 9.095581 5.877643

41 H 8.007478 8.879177 8.268521 9.095581 5.877643

42 H 7.701877 8.761219 8.389910 9.396289 6.411432

43 H 2.155561 3.313432 4.338781 5.628930 5.893638

44 H 2.155561 3.313432 4.338781 5.628930 5.893638

45 H 2.147902 2.755522 4.120307 5.242034 6.392542

26 27 28 29 30

26 C 0.000000

27 H 2.987027 0.000000

28 C 7.925234 9.456266 0.000000

29 H 5.284502 7.388057 2.979487 0.000000

30 C 7.931542 5.278418 11.218126 10.425445 0.000000

31 H 9.461165 7.377004 10.425445 10.454098 2.979487

32 C 11.206741 10.403494 7.931542 9.461165 7.925234

33 H 10.403494 10.426840 5.278418 7.377004 9.456266

34 H 1.092514 2.724355 9.016878 6.363787 7.959162

35 H 1.095494 3.744281 7.687718 4.962988 8.561081

36 H 1.095494 3.744281 7.687718 4.962988 8.561081

37 H 8.543780 9.952306 1.094897 3.734325 11.437559

38 H 8.543780 9.952306 1.094897 3.734325 11.437559

39 H 7.974529 9.807939 1.091792 2.735244 11.997670

40 H 7.674160 4.940089 11.437559 10.478181 1.094897

41 H 7.674160 4.940089 11.437559 10.478181 1.094897

42 H 9.023044 6.354269 11.997670 11.374333 1.091792

43 H 11.448378 10.479017 8.561081 9.974105 7.687718

44 H 11.448378 10.479017 8.561081 9.974105 7.687718

45 H 11.972097 11.343129 7.959162 9.791603 9.016878

31 32 33 34 35

31 H 0.000000

32 C 5.284502 0.000000

33 H 7.388057 2.987027 0.000000

34 H 9.791603 11.972097 11.343129 0.000000

35 H 9.974105 11.448378 10.479017 1.767339 0.000000

36 H 9.974105 11.448378 10.479017 1.767339 1.754408

37 H 10.478181 7.674160 4.940089 9.627992 8.232831

38 H 10.478181 7.674160 4.940089 9.627992 8.417602

39 H 11.374333 9.023044 6.354269 9.062731 7.657531

40 H 3.734325 8.543780 9.952306 7.623931 8.228444

41 H 3.734325 8.543780 9.952306 7.623931 8.413312

42 H 2.735244 7.974529 9.807939 9.044833 9.645987

43 H 4.962988 1.095494 3.744281 12.168633 11.655983

44 H 4.962988 1.095494 3.744281 12.168633 11.787276

45 H 6.363787 1.092514 2.724355 12.785084 12.168633

36 37 38 39 40

36 H 0.000000

37 H 8.417602 0.000000

38 H 8.232831 1.753598 0.000000

39 H 7.657531 1.771720 1.771720 0.000000

40 H 8.413312 11.623754 11.755287 12.172400 0.000000

41 H 8.228444 11.755287 11.623754 12.172400 1.753598

42 H 9.645987 12.172400 12.172400 12.822864 1.771720

43 H 11.787276 8.228444 8.413312 9.645987 8.232831

44 H 11.655983 8.413312 8.228444 9.645987 8.417602

45 H 12.168633 7.623931 7.623931 9.044833 9.627992

41 42 43 44 45

41 H 0.000000

42 H 1.771720 0.000000

43 H 8.417602 7.657531 0.000000

44 H 8.232831 7.657531 1.754408 0.000000

45 H 9.627992 9.062731 1.767339 1.767339 0.000000

Stoichiometry C20H16N8Zn(1-,2)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=3 Diff= 1.57D-16

Largest Abelian subgroup C2H NOp 4

Largest concise Abelian subgroup C2H 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 -2.948481 0.654969 0.000000

2 7 0 -1.987918 -0.316570 0.000000

3 6 0 -2.590893 -1.543911 0.000000

4 6 0 -4.021983 -1.356746 0.000000

5 6 0 -4.233713 0.015731 0.000000

6 7 0 -1.972248 -2.760402 0.000000

7 6 0 -0.661775 -2.941027 0.000000

8 7 0 0.316496 -1.981449 0.000000

9 6 0 1.546193 -2.579782 0.000000

10 6 0 1.343298 -4.049252 0.000000

11 6 0 0.000000 -4.253427 0.000000

12 7 0 -2.736350 2.005625 0.000000

13 6 0 -1.343298 4.049252 0.000000

14 6 0 0.000000 4.253427 0.000000

15 6 0 0.661775 2.941027 0.000000

16 7 0 -0.316496 1.981449 0.000000

17 6 0 -1.546193 2.579782 0.000000

18 7 0 1.972248 2.760402 0.000000

19 7 0 1.987918 0.316570 0.000000

20 6 0 2.590893 1.543911 0.000000

21 6 0 4.021983 1.356746 0.000000

22 6 0 4.233713 -0.015731 0.000000

23 6 0 2.948481 -0.654969 0.000000

24 7 0 2.736350 -2.005625 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -5.037526 -2.453791 0.000000

27 1 0 -5.186459 0.529521 0.000000

28 6 0 2.452270 -5.044597 0.000000

29 1 0 -0.523119 -5.200806 0.000000

30 6 0 -2.452270 5.044597 0.000000

31 1 0 0.523119 5.200806 0.000000

32 6 0 5.037526 2.453791 0.000000

33 1 0 5.186459 -0.529521 0.000000

34 1 0 -6.053889 -2.053051 0.000000

35 1 0 -4.934003 -3.101790 0.877204

36 1 0 -4.934003 -3.101790 -0.877204

37 1 0 3.095835 -4.918711 0.876799

38 1 0 3.095835 -4.918711 -0.876799

39 1 0 2.071117 -6.067696 0.000000

40 1 0 -3.095835 4.918711 0.876799

41 1 0 -3.095835 4.918711 -0.876799

42 1 0 -2.071117 6.067696 0.000000

43 1 0 4.934003 3.101790 0.877204

44 1 0 4.934003 3.101790 -0.877204

45 1 0 6.053889 2.053051 0.000000

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

Rotational constants (GHZ): 0.1827855 0.1817031 0.0913256

Leave Link 202 at Tue Sep 17 14:08:41 2019, MaxMem= 2415919104 cpu: 0.1

(Enter /home/blab/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 (BU) (AG) (BU) (AG) (BU) (AG) (BU) (AG) (BU) (AG)

(BU) (AG) (BU) (AG) (BU) (AG) (BU) (AG) (BU) (AG)

(BU) (AG) (BU) (AG) (BU) (AG) (BU) (AG) (AG) (BU)

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The electronic state is 2-BG.

Alpha occ. eigenvalues -- -14.29542 -14.29542 -14.29539 -14.29539 -14.28338

Alpha occ. eigenvalues -- -14.28338 -14.28307 -14.28307 -10.22696 -10.22696

Alpha occ. eigenvalues -- -10.22555 -10.22555 -10.21402 -10.21402 -10.21161

Alpha occ. eigenvalues -- -10.21161 -10.17669 -10.17669 -10.16178 -10.16178

Alpha occ. eigenvalues -- -10.16144 -10.16144 -10.15796 -10.15796 -10.15367

Alpha occ. eigenvalues -- -10.15367 -10.14816 -10.14816 -0.97997 -0.96821

Alpha occ. eigenvalues -- -0.96333 -0.93831 -0.91754 -0.87894 -0.87358

Alpha occ. eigenvalues -- -0.84395 -0.78445 -0.78186 -0.77133 -0.77097

Alpha occ. eigenvalues -- -0.73042 -0.70289 -0.70089 -0.69132 -0.67650

Alpha occ. eigenvalues -- -0.66408 -0.65931 -0.60841 -0.59137 -0.57035

Alpha occ. eigenvalues -- -0.56095 -0.55692 -0.55182 -0.54956 -0.54172

Alpha occ. eigenvalues -- -0.54116 -0.52920 -0.52385 -0.51755 -0.51112

Alpha occ. eigenvalues -- -0.50060 -0.49009 -0.48655 -0.46996 -0.46719

Alpha occ. eigenvalues -- -0.44419 -0.43214 -0.43047 -0.42831 -0.42449

Alpha occ. eigenvalues -- -0.41708 -0.41635 -0.41378 -0.39798 -0.39604

Alpha occ. eigenvalues -- -0.39183 -0.38657 -0.38177 -0.38124 -0.37967

Alpha occ. eigenvalues -- -0.37441 -0.36373 -0.36326 -0.35955 -0.35666

Alpha occ. eigenvalues -- -0.35571 -0.35214 -0.31151 -0.30782 -0.30638

Alpha occ. eigenvalues -- -0.30093 -0.29073 -0.26200 -0.26138 -0.24987

Alpha occ. eigenvalues -- -0.24480 -0.24083 -0.23787 -0.23643 -0.22980

Alpha occ. eigenvalues -- -0.22910 -0.19765 -0.13543

Alpha virt. eigenvalues -- -0.08616 -0.04155 0.03993 0.04424 0.04961

Alpha virt. eigenvalues -- 0.05019 0.05987 0.06026 0.06138 0.07246

Alpha virt. eigenvalues -- 0.07333 0.07501 0.08565 0.08616 0.09743

Alpha virt. eigenvalues -- 0.10417 0.10551 0.10765 0.11056 0.11387

Alpha virt. eigenvalues -- 0.12483 0.12524 0.13340 0.14027 0.14097

Alpha virt. eigenvalues -- 0.14159 0.14161 0.14581 0.14716 0.14943

Alpha virt. eigenvalues -- 0.19587 0.21222 0.21530 0.21839 0.22352

Alpha virt. eigenvalues -- 0.22842 0.22967 0.23179 0.23594 0.23980

Alpha virt. eigenvalues -- 0.24367 0.24464 0.25599 0.27847 0.28649

Alpha virt. eigenvalues -- 0.28743 0.29181 0.29856 0.30716 0.31082

Alpha virt. eigenvalues -- 0.31740 0.31945 0.31948 0.32001 0.32471

Alpha virt. eigenvalues -- 0.32902 0.33199 0.33266 0.33342 0.33671

Alpha virt. eigenvalues -- 0.35886 0.36393 0.36721 0.37205 0.38857

Alpha virt. eigenvalues -- 0.39310 0.39487 0.40319 0.40334 0.40587

Alpha virt. eigenvalues -- 0.41502 0.41641 0.42006 0.42894 0.42938

Alpha virt. eigenvalues -- 0.44720 0.45009 0.45183 0.45376 0.45470

Alpha virt. eigenvalues -- 0.46670 0.47226 0.47537 0.48839 0.49336

Alpha virt. eigenvalues -- 0.49985 0.50158 0.51060 0.51141 0.51199

Alpha virt. eigenvalues -- 0.51451 0.52657 0.52780 0.52959 0.52997

Alpha virt. eigenvalues -- 0.54203 0.54771 0.54910 0.55059 0.55427

Alpha virt. eigenvalues -- 0.57547 0.57692 0.58022 0.58024 0.58463

Alpha virt. eigenvalues -- 0.58655 0.58806 0.59086 0.59335 0.59699

Alpha virt. eigenvalues -- 0.60200 0.60431 0.61376 0.61449 0.61509

Alpha virt. eigenvalues -- 0.63228 0.64010 0.64464 0.64710 0.64741

Alpha virt. eigenvalues -- 0.65230 0.65340 0.66449 0.66519 0.66602

Alpha virt. eigenvalues -- 0.69424 0.69551 0.69773 0.70071 0.70402

Alpha virt. eigenvalues -- 0.70580 0.70873 0.71886 0.72749 0.72868

Alpha virt. eigenvalues -- 0.74579 0.74956 0.75437 0.76271 0.76901

Alpha virt. eigenvalues -- 0.77420 0.77566 0.79021 0.79868 0.80300

Alpha virt. eigenvalues -- 0.81106 0.81725 0.82026 0.82232 0.82415

Alpha virt. eigenvalues -- 0.82602 0.83560 0.83655 0.83917 0.86288

Alpha virt. eigenvalues -- 0.86673 0.87039 0.87888 0.89909 0.90117

Alpha virt. eigenvalues -- 0.90647 0.91217 0.95811 0.98025 0.98844

Alpha virt. eigenvalues -- 0.98887 0.99319 1.01101 1.01444 1.02892

Alpha virt. eigenvalues -- 1.05091 1.05251 1.05321 1.06402 1.06858

Alpha virt. eigenvalues -- 1.08216 1.09515 1.10410 1.11177 1.11956

Alpha virt. eigenvalues -- 1.12558 1.15013 1.15057 1.15262 1.15684

Alpha virt. eigenvalues -- 1.16005 1.16095 1.16589 1.16666 1.17662

Alpha virt. eigenvalues -- 1.19645 1.20573 1.20762 1.21235 1.22440

Alpha virt. eigenvalues -- 1.23226 1.23978 1.24992 1.25705 1.29334

Alpha virt. eigenvalues -- 1.30889 1.31092 1.31107 1.32825 1.38461

Alpha virt. eigenvalues -- 1.38714 1.38984 1.40624 1.40940 1.42704

Alpha virt. eigenvalues -- 1.42861 1.42965 1.43701 1.43963 1.45776

Alpha virt. eigenvalues -- 1.47308 1.51153 1.51418 1.51706 1.51713

Alpha virt. eigenvalues -- 1.51776 1.52103 1.52124 1.53357 1.53455

Alpha virt. eigenvalues -- 1.53659 1.54310 1.55637 1.56213 1.56449

Alpha virt. eigenvalues -- 1.57387 1.57388 1.57647 1.58665 1.60205

Alpha virt. eigenvalues -- 1.61640 1.62214 1.63367 1.63739 1.64433

Alpha virt. eigenvalues -- 1.64760 1.65465 1.68698 1.70045 1.70159

Alpha virt. eigenvalues -- 1.70862 1.70864 1.71134 1.71246 1.72714

Alpha virt. eigenvalues -- 1.73282 1.75685 1.76057 1.77774 1.78421

Alpha virt. eigenvalues -- 1.79414 1.81240 1.81381 1.81726 1.82185

Alpha virt. eigenvalues -- 1.86486 1.88250 1.88498 1.89419 1.90248

Alpha virt. eigenvalues -- 1.92254 1.92320 1.93540 1.94345 1.96279

Alpha virt. eigenvalues -- 1.97373 1.98017 1.99241 1.99421 2.01454

Alpha virt. eigenvalues -- 2.01504 2.02781 2.02790 2.03468 2.03609

Alpha virt. eigenvalues -- 2.04011 2.05018 2.07192 2.08597 2.10209

Alpha virt. eigenvalues -- 2.10647 2.12238 2.14617 2.15022 2.17026

Alpha virt. eigenvalues -- 2.17644 2.17966 2.19520 2.20292 2.22364

Alpha virt. eigenvalues -- 2.28815 2.30302 2.30557 2.30711 2.31288

Alpha virt. eigenvalues -- 2.32262 2.34706 2.35486 2.35700 2.35854

Alpha virt. eigenvalues -- 2.36096 2.36677 2.39263 2.39360 2.40312

Alpha virt. eigenvalues -- 2.40549 2.41235 2.41640 2.41903 2.45709

Alpha virt. eigenvalues -- 2.49015 2.49382 2.49811 2.49847 2.50085

Alpha virt. eigenvalues -- 2.50098 2.50925 2.51063 2.56835 2.56883

Alpha virt. eigenvalues -- 2.57843 2.58190 2.59680 2.60291 2.61370

Alpha virt. eigenvalues -- 2.61971 2.62807 2.65118 2.65401 2.66599

Alpha virt. eigenvalues -- 2.68521 2.68907 2.72379 2.72659 2.73697

Alpha virt. eigenvalues -- 2.73805 2.74005 2.74564 2.77760 2.78549

Alpha virt. eigenvalues -- 2.78783 2.82179 2.85044 2.85993 2.86126

Alpha virt. eigenvalues -- 2.86386 2.86519 2.86861 2.86929 2.86941

Alpha virt. eigenvalues -- 2.93961 2.94338 2.94896 2.95934 2.97517

Alpha virt. eigenvalues -- 2.98785 3.00075 3.04013 3.05681 3.05785

Alpha virt. eigenvalues -- 3.07403 3.08442 3.13633 3.13808 3.14343

Alpha virt. eigenvalues -- 3.14467 3.14745 3.15197 3.15968 3.17291

Alpha virt. eigenvalues -- 3.17630 3.18364 3.19379 3.19605 3.22332

Alpha virt. eigenvalues -- 3.22726 3.23314 3.24355 3.26444 3.28636

Alpha virt. eigenvalues -- 3.29964 3.30628 3.31161 3.32158 3.33937

Alpha virt. eigenvalues -- 3.38597 3.39585 3.40243 3.41406 3.41870

Alpha virt. eigenvalues -- 3.55734 3.58947 3.60182 3.71910 3.74100

Alpha virt. eigenvalues -- 3.74330 3.74392 3.77917 3.79694 3.79915

Alpha virt. eigenvalues -- 3.80835 3.80842 3.82948 3.83718 3.83733

Alpha virt. eigenvalues -- 3.88907 3.89294 3.89487 3.90070 3.93023

Alpha virt. eigenvalues -- 4.06350 4.06906 4.06945 4.07695 4.13244

Alpha virt. eigenvalues -- 4.14142 4.14729 4.20919 4.30597 4.38074

Alpha virt. eigenvalues -- 4.38333 4.40658 4.48281 4.53330 4.63146

Alpha virt. eigenvalues -- 4.63827 5.02432 5.05247 5.06078 5.14122

Alpha virt. eigenvalues -- 5.16929 5.34026 5.34855 5.51068 7.79814

Alpha virt. eigenvalues -- 7.79918 7.91004 7.96711 8.24150 11.20607

Alpha virt. eigenvalues -- 23.45011 23.46988 23.48354 23.49175 23.67419

Alpha virt. eigenvalues -- 23.68081 23.68223 23.68363 23.85154 23.85201

Alpha virt. eigenvalues -- 23.88288 23.88733 23.89614 23.90023 23.90796

Alpha virt. eigenvalues -- 23.91497 24.09005 24.09049 24.14581 24.14739

Alpha virt. eigenvalues -- 35.58536 35.62416 35.63225 35.63619 35.69547

Alpha virt. eigenvalues -- 35.70452 35.70492 35.70545

Beta occ. eigenvalues -- -14.29385 -14.29385 -14.29381 -14.29381 -14.28401

Beta occ. eigenvalues -- -14.28401 -14.28146 -14.28146 -10.22722 -10.22722

Beta occ. eigenvalues -- -10.22587 -10.22587 -10.21225 -10.21225 -10.20977

Beta occ. eigenvalues -- -10.20977 -10.17677 -10.17677 -10.16183 -10.16183

Beta occ. eigenvalues -- -10.16018 -10.16018 -10.15796 -10.15796 -10.15375

Beta occ. eigenvalues -- -10.15375 -10.14738 -10.14738 -0.97769 -0.96625

Beta occ. eigenvalues -- -0.96060 -0.93641 -0.91407 -0.87623 -0.87025

Beta occ. eigenvalues -- -0.84083 -0.78369 -0.78118 -0.76953 -0.76910

Beta occ. eigenvalues -- -0.72804 -0.70215 -0.69818 -0.69042 -0.67555

Beta occ. eigenvalues -- -0.66147 -0.65888 -0.60677 -0.58906 -0.56982

Beta occ. eigenvalues -- -0.56040 -0.55654 -0.55124 -0.54760 -0.54116

Beta occ. eigenvalues -- -0.54106 -0.52847 -0.52315 -0.51595 -0.50967

Beta occ. eigenvalues -- -0.49975 -0.48937 -0.48533 -0.46914 -0.46595

Beta occ. eigenvalues -- -0.43941 -0.43016 -0.42994 -0.42428 -0.42151

Beta occ. eigenvalues -- -0.41574 -0.41440 -0.41326 -0.39642 -0.39384

Beta occ. eigenvalues -- -0.38860 -0.38599 -0.38142 -0.38088 -0.37918

Beta occ. eigenvalues -- -0.36907 -0.36298 -0.36208 -0.35613 -0.35521

Beta occ. eigenvalues -- -0.35159 -0.35117 -0.31007 -0.30597 -0.30028

Beta occ. eigenvalues -- -0.29072 -0.28848 -0.26010 -0.25955 -0.24629

Beta occ. eigenvalues -- -0.24300 -0.23641 -0.23555 -0.22804 -0.22506

Beta occ. eigenvalues -- -0.22356 -0.18328

Beta virt. eigenvalues -- -0.09057 -0.08614 -0.02915 0.04039 0.04972

Beta virt. eigenvalues -- 0.05071 0.05191 0.06159 0.06281 0.06857

Beta virt. eigenvalues -- 0.07343 0.07518 0.07680 0.08570 0.08644

Beta virt. eigenvalues -- 0.09759 0.10422 0.10581 0.10793 0.11687

Beta virt. eigenvalues -- 0.11967 0.12946 0.13140 0.13347 0.14032

Beta virt. eigenvalues -- 0.14177 0.14180 0.14191 0.14783 0.15172

Beta virt. eigenvalues -- 0.15227 0.19750 0.21293 0.21600 0.21943

Beta virt. eigenvalues -- 0.22488 0.22894 0.23208 0.23272 0.23678

Beta virt. eigenvalues -- 0.24053 0.24456 0.24620 0.25831 0.27942

Beta virt. eigenvalues -- 0.28728 0.28852 0.29246 0.29960 0.30866

Beta virt. eigenvalues -- 0.31227 0.31815 0.31976 0.32008 0.32170

Beta virt. eigenvalues -- 0.32624 0.33046 0.33257 0.33375 0.33459

Beta virt. eigenvalues -- 0.33809 0.35927 0.36465 0.36871 0.37350

Beta virt. eigenvalues -- 0.39022 0.39377 0.39613 0.40436 0.40469

Beta virt. eigenvalues -- 0.41028 0.41517 0.41730 0.42195 0.43021

Beta virt. eigenvalues -- 0.43150 0.44827 0.45189 0.45312 0.45501

Beta virt. eigenvalues -- 0.45870 0.46799 0.47474 0.47734 0.48926

Beta virt. eigenvalues -- 0.49440 0.50194 0.50266 0.51153 0.51260

Beta virt. eigenvalues -- 0.51287 0.51575 0.52925 0.53058 0.53071

Beta virt. eigenvalues -- 0.53255 0.54440 0.54849 0.54948 0.55150

Beta virt. eigenvalues -- 0.55467 0.57622 0.57773 0.58069 0.58085

Beta virt. eigenvalues -- 0.58523 0.58704 0.58992 0.59155 0.59370

Beta virt. eigenvalues -- 0.59764 0.60213 0.60522 0.61459 0.61541

Beta virt. eigenvalues -- 0.61640 0.63309 0.64048 0.64520 0.64858

Beta virt. eigenvalues -- 0.65026 0.65344 0.65472 0.66523 0.66573

Beta virt. eigenvalues -- 0.66687 0.69473 0.69838 0.69892 0.70091

Beta virt. eigenvalues -- 0.70554 0.70949 0.71058 0.72002 0.72896

Beta virt. eigenvalues -- 0.73227 0.74751 0.75108 0.75524 0.76347

Beta virt. eigenvalues -- 0.76995 0.77517 0.77639 0.79115 0.79965

Beta virt. eigenvalues -- 0.80384 0.81381 0.81860 0.82494 0.82633

Beta virt. eigenvalues -- 0.82693 0.82703 0.83651 0.83719 0.84000

Beta virt. eigenvalues -- 0.86347 0.86760 0.87135 0.87943 0.89983

Beta virt. eigenvalues -- 0.90175 0.90902 0.91318 0.95918 0.98090

Beta virt. eigenvalues -- 0.98921 0.98922 0.99402 1.01131 1.01611

Beta virt. eigenvalues -- 1.03124 1.05172 1.05385 1.05599 1.06522

Beta virt. eigenvalues -- 1.06941 1.08387 1.09572 1.10435 1.11671

Beta virt. eigenvalues -- 1.12030 1.12762 1.15079 1.15132 1.15313

Beta virt. eigenvalues -- 1.15790 1.16074 1.16171 1.16985 1.17257

Beta virt. eigenvalues -- 1.18143 1.19755 1.20649 1.20809 1.21618

Beta virt. eigenvalues -- 1.22542 1.23493 1.24308 1.25051 1.25771

Beta virt. eigenvalues -- 1.29422 1.31014 1.31170 1.31380 1.32963

Beta virt. eigenvalues -- 1.38749 1.39049 1.39156 1.40987 1.41051

Beta virt. eigenvalues -- 1.42783 1.42960 1.43242 1.43901 1.44184

Beta virt. eigenvalues -- 1.45855 1.47470 1.51210 1.51491 1.51709

Beta virt. eigenvalues -- 1.51778 1.51781 1.52166 1.52184 1.53455

Beta virt. eigenvalues -- 1.53510 1.53725 1.54387 1.55764 1.56321

Beta virt. eigenvalues -- 1.56537 1.57408 1.57535 1.57888 1.58775

Beta virt. eigenvalues -- 1.60450 1.61753 1.62216 1.63656 1.63778

Beta virt. eigenvalues -- 1.64491 1.64932 1.65617 1.68783 1.70147

Beta virt. eigenvalues -- 1.70242 1.70932 1.71053 1.71198 1.71367

Beta virt. eigenvalues -- 1.72806 1.73341 1.75775 1.76566 1.77895

Beta virt. eigenvalues -- 1.78536 1.79799 1.81312 1.81442 1.81904

Beta virt. eigenvalues -- 1.82373 1.86582 1.88376 1.88613 1.89660

Beta virt. eigenvalues -- 1.90393 1.92344 1.92381 1.94046 1.94700

Beta virt. eigenvalues -- 1.96367 1.97583 1.98058 1.99559 1.99641

Beta virt. eigenvalues -- 2.01934 2.01995 2.02784 2.02806 2.03921

Beta virt. eigenvalues -- 2.03924 2.04143 2.05061 2.07332 2.08677

Beta virt. eigenvalues -- 2.10560 2.10786 2.12369 2.14971 2.15395

Beta virt. eigenvalues -- 2.17250 2.17774 2.18285 2.19753 2.20351

Beta virt. eigenvalues -- 2.22745 2.28899 2.30571 2.30771 2.30799

Beta virt. eigenvalues -- 2.31331 2.32487 2.35149 2.35718 2.35732

Beta virt. eigenvalues -- 2.35875 2.36144 2.36702 2.39455 2.39558

Beta virt. eigenvalues -- 2.40361 2.40861 2.41535 2.41782 2.42132

Beta virt. eigenvalues -- 2.45825 2.49114 2.49512 2.49982 2.50067

Beta virt. eigenvalues -- 2.50230 2.50300 2.51175 2.51232 2.56868

Beta virt. eigenvalues -- 2.57030 2.58231 2.58356 2.59797 2.60464

Beta virt. eigenvalues -- 2.61594 2.62016 2.63371 2.65499 2.65566

Beta virt. eigenvalues -- 2.66825 2.68891 2.68995 2.72764 2.73020

Beta virt. eigenvalues -- 2.73966 2.74073 2.74183 2.74784 2.78115

Beta virt. eigenvalues -- 2.78889 2.79155 2.82454 2.85448 2.86185

Beta virt. eigenvalues -- 2.86367 2.86590 2.86874 2.86914 2.87026

Beta virt. eigenvalues -- 2.87467 2.94012 2.94414 2.94949 2.96199

Beta virt. eigenvalues -- 2.97573 2.98783 3.00804 3.04474 3.05722

Beta virt. eigenvalues -- 3.05808 3.07489 3.08513 3.13674 3.13843

Beta virt. eigenvalues -- 3.14348 3.14573 3.14813 3.15242 3.16084

Beta virt. eigenvalues -- 3.17319 3.17697 3.18422 3.19418 3.19686

Beta virt. eigenvalues -- 3.22432 3.22789 3.23394 3.24427 3.26500

Beta virt. eigenvalues -- 3.28692 3.30003 3.30702 3.31234 3.32188

Beta virt. eigenvalues -- 3.34071 3.38673 3.39623 3.40247 3.41541

Beta virt. eigenvalues -- 3.41976 3.55845 3.59012 3.60300 3.72004

Beta virt. eigenvalues -- 3.74203 3.74404 3.74511 3.78007 3.79750

Beta virt. eigenvalues -- 3.80070 3.80906 3.80974 3.83601 3.83936

Beta virt. eigenvalues -- 3.84441 3.89235 3.89997 3.90179 3.90444

Beta virt. eigenvalues -- 3.93346 4.06379 4.06959 4.07101 4.07892

Beta virt. eigenvalues -- 4.13363 4.14202 4.14911 4.21046 4.30716

Beta virt. eigenvalues -- 4.38224 4.38506 4.40828 4.48404 4.53406

Beta virt. eigenvalues -- 4.63286 4.63854 5.02594 5.05343 5.06318

Beta virt. eigenvalues -- 5.14270 5.17124 5.34191 5.35033 5.51241

Beta virt. eigenvalues -- 7.79813 7.79965 7.91003 7.96716 8.24156

Beta virt. eigenvalues -- 11.20620 23.45038 23.46982 23.48435 23.49225

Beta virt. eigenvalues -- 23.67448 23.68134 23.68221 23.68383 23.85158

Beta virt. eigenvalues -- 23.85180 23.88479 23.88887 23.89723 23.90123

Beta virt. eigenvalues -- 23.90863 23.91565 24.09128 24.09171 24.14575

Beta virt. eigenvalues -- 24.14734 35.58646 35.62584 35.63197 35.63652

Beta virt. eigenvalues -- 35.69714 35.70592 35.70652 35.70674

Condensed to atoms (all electrons):

1 2 3 4 5 6

1 C 4.700520 0.411127 -0.145344 -0.062046 0.465269 -0.001269

2 N 0.411127 7.100454 0.383096 -0.068571 -0.102550 -0.080224

3 C -0.145344 0.383096 4.730770 0.472944 -0.076483 0.519635

4 C -0.062046 -0.068571 0.472944 5.089463 0.578888 -0.081750

5 C 0.465269 -0.102550 -0.076483 0.578888 5.194834 0.005776

6 N -0.001269 -0.080224 0.519635 -0.081750 0.005776 6.616541

7 C -0.000603 -0.001764 -0.106474 0.002323 -0.000413 0.556634

8 N 0.000278 -0.022050 -0.003182 -0.000001 -0.000199 -0.082659

9 C -0.000009 0.000255 -0.000823 0.000015 -0.000003 0.000633

10 C -0.000003 -0.000065 0.000135 0.000021 0.000000 0.003279

11 C 0.000018 0.000209 0.004346 -0.000400 0.000011 -0.044245

12 N 0.474403 -0.073130 0.000941 0.004487 -0.047541 -0.000145

13 C 0.004619 -0.000153 0.000019 0.000020 -0.000462 -0.000000

14 C -0.000306 -0.000189 -0.000003 0.000000 0.000010 -0.000000

15 C -0.001021 0.000424 -0.000009 -0.000003 0.000019 -0.000001

16 N -0.002309 -0.021985 0.000088 -0.000080 0.000436 -0.000005

17 C -0.107307 -0.003089 -0.000468 0.000126 0.003211 -0.000023

18 N -0.000024 -0.000006 -0.000001 -0.000000 -0.000000 0.000000

19 N 0.000155 -0.002911 0.000207 0.000002 0.000003 -0.000006

20 C -0.000051 0.000207 -0.000011 -0.000000 -0.000000 -0.000001

21 C -0.000000 0.000002 -0.000000 0.000000 -0.000000 -0.000000

22 C -0.000000 0.000003 -0.000000 -0.000000 0.000000 -0.000000

23 C -0.000004 0.000155 -0.000051 -0.000000 -0.000000 -0.000024

24 N -0.000001 -0.000006 -0.000031 -0.000000 -0.000000 -0.000158

25 Zn -0.016385 0.129604 -0.017915 -0.000562 0.000330 -0.005669

26 C 0.010329 0.009919 -0.073690 0.260459 -0.060338 0.015357

27 H -0.053905 0.007376 0.010489 -0.047350 0.396831 -0.000020

28 C 0.000000 0.000001 0.000002 -0.000000 0.000000 -0.000019

29 H 0.000002 0.000083 -0.000115 -0.000180 -0.000006 0.007631

30 C -0.000446 0.000066 0.000000 -0.000001 -0.000026 0.000000

31 H 0.000013 0.000001 0.000000 0.000000 -0.000000 -0.000000

32 C 0.000000 -0.000000 0.000000 -0.000000 -0.000000 -0.000000

33 H -0.000000 0.000000 -0.000000 -0.000000 -0.000000 0.000000

34 H 0.000222 -0.000244 0.006085 -0.043360 -0.005191 0.000108

35 H -0.000018 0.000437 -0.005916 -0.047126 0.000101 0.004586

36 H -0.000018 0.000437 -0.005916 -0.047126 0.000101 0.004586

37 H 0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000010

38 H 0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000010

39 H -0.000000 -0.000000 0.000001 0.000000 0.000000 -0.000010

40 H -0.000051 0.000015 -0.000000 0.000000 -0.000020 0.000000

41 H -0.000051 0.000015 -0.000000 0.000000 -0.000020 0.000000

42 H 0.000043 0.000000 0.000000 0.000000 -0.000001 0.000000

43 H 0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000000

44 H 0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000000

45 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000000

7 8 9 10 11 12

1 C -0.000603 0.000278 -0.000009 -0.000003 0.000018 0.474403

2 N -0.001764 -0.022050 0.000255 -0.000065 0.000209 -0.073130

3 C -0.106474 -0.003182 -0.000823 0.000135 0.004346 0.000941

4 C 0.002323 -0.000001 0.000015 0.000021 -0.000400 0.004487

5 C -0.000413 -0.000199 -0.000003 0.000000 0.000011 -0.047541

6 N 0.556634 -0.082659 0.000633 0.003279 -0.044245 -0.000145

7 C 4.632190 0.400552 -0.131429 -0.056621 0.405680 -0.000016

8 N 0.400552 7.161834 0.377516 -0.063053 -0.101969 -0.000004

9 C -0.131429 0.377516 4.658861 0.398997 -0.068084 -0.000001

10 C -0.056621 -0.063053 0.398997 5.080439 0.625789 -0.000000

11 C 0.405680 -0.101969 -0.068084 0.625789 5.160601 -0.000000

12 N -0.000016 -0.000004 -0.000001 -0.000000 -0.000000 6.615620

13 C -0.000000 0.000002 -0.000000 0.000000 -0.000000 -0.079130

14 C -0.000000 0.000003 -0.000000 -0.000000 0.000000 0.004811

15 C -0.000003 0.000163 -0.000056 -0.000000 -0.000000 -0.001780

16 N 0.000163 -0.003160 0.000215 0.000002 0.000003 -0.090268

17 C -0.000056 0.000215 -0.000010 -0.000000 -0.000000 0.602625

18 N -0.000001 -0.000005 -0.000023 -0.000000 -0.000000 -0.000158

19 N 0.000424 -0.021985 -0.003089 -0.000153 -0.000189 -0.000006

20 C -0.000009 0.000088 -0.000468 0.000019 -0.000003 -0.000031

21 C -0.000003 -0.000080 0.000126 0.000020 0.000000 -0.000000

22 C 0.000019 0.000436 0.003211 -0.000462 0.000010 -0.000000

23 C -0.001021 -0.002309 -0.107307 0.004619 -0.000306 -0.000001

24 N -0.001780 -0.090268 0.602625 -0.079130 0.004811 0.000000

25 Zn -0.016828 0.127782 -0.018407 -0.000267 0.000203 -0.005796

26 C -0.000068 0.000067 0.000001 -0.000001 -0.000036 -0.000026

27 H 0.000008 0.000002 0.000000 0.000000 -0.000000 0.006950

28 C 0.010558 0.009879 -0.068459 0.256587 -0.060337 -0.000000

29 H -0.050383 0.006871 0.010448 -0.046241 0.394013 0.000000

30 C 0.000000 -0.000000 0.000000 -0.000000 -0.000000 0.016158

31 H 0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000004

32 C 0.000000 0.000001 -0.000000 -0.000000 0.000000 0.000000

33 H 0.000002 0.000087 0.000079 -0.000181 -0.000006 -0.000000

34 H 0.000044 0.000000 0.000000 0.000000 -0.000001 -0.000012

35 H 0.000102 0.000012 -0.000000 -0.000000 -0.000021 0.000007

36 H 0.000102 0.000012 -0.000000 -0.000000 -0.000021 0.000007

37 H -0.000062 0.000450 -0.004376 -0.046224 -0.000824 -0.000000

38 H -0.000062 0.000450 -0.004376 -0.046224 -0.000824 -0.000000

39 H 0.000194 -0.000251 0.005952 -0.042159 -0.005079 -0.000000

40 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.004897

41 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.004897

42 H 0.000000 -0.000000 0.000000 0.000000 0.000000 0.000119

43 H 0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000000

44 H 0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000000

45 H -0.000000 -0.000000 0.000001 0.000000 0.000000 0.000000

13 14 15 16 17 18

1 C 0.004619 -0.000306 -0.001021 -0.002309 -0.107307 -0.000024

2 N -0.000153 -0.000189 0.000424 -0.021985 -0.003089 -0.000006

3 C 0.000019 -0.000003 -0.000009 0.000088 -0.000468 -0.000001

4 C 0.000020 0.000000 -0.000003 -0.000080 0.000126 -0.000000

5 C -0.000462 0.000010 0.000019 0.000436 0.003211 -0.000000

6 N -0.000000 -0.000000 -0.000001 -0.000005 -0.000023 0.000000

7 C -0.000000 -0.000000 -0.000003 0.000163 -0.000056 -0.000001

8 N 0.000002 0.000003 0.000163 -0.003160 0.000215 -0.000005

9 C -0.000000 -0.000000 -0.000056 0.000215 -0.000010 -0.000023

10 C 0.000000 -0.000000 -0.000000 0.000002 -0.000000 -0.000000

11 C -0.000000 0.000000 -0.000000 0.000003 -0.000000 -0.000000

12 N -0.079130 0.004811 -0.001780 -0.090268 0.602625 -0.000158

13 C 5.080439 0.625789 -0.056621 -0.063053 0.398997 0.003279

14 C 0.625789 5.160601 0.405680 -0.101969 -0.068084 -0.044245

15 C -0.056621 0.405680 4.632190 0.400552 -0.131429 0.556634

16 N -0.063053 -0.101969 0.400552 7.161834 0.377516 -0.082659

17 C 0.398997 -0.068084 -0.131429 0.377516 4.658861 0.000633

18 N 0.003279 -0.044245 0.556634 -0.082659 0.000633 6.616541

19 N -0.000065 0.000209 -0.001764 -0.022050 0.000255 -0.080224

20 C 0.000135 0.004346 -0.106474 -0.003182 -0.000823 0.519635

21 C 0.000021 -0.000400 0.002323 -0.000001 0.000015 -0.081750

22 C 0.000000 0.000011 -0.000413 -0.000199 -0.000003 0.005776

23 C -0.000003 0.000018 -0.000603 0.000278 -0.000009 -0.001269

24 N -0.000000 -0.000000 -0.000016 -0.000004 -0.000001 -0.000145

25 Zn -0.000267 0.000203 -0.016828 0.127782 -0.018407 -0.005669

26 C -0.000000 0.000000 0.000000 0.000001 -0.000000 -0.000000

27 H -0.000181 -0.000006 0.000002 0.000087 0.000079 0.000000

28 C -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

29 H -0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000000

30 C 0.256587 -0.060337 0.010558 0.009879 -0.068459 -0.000019

31 H -0.046241 0.394013 -0.050383 0.006871 0.010448 0.007631

32 C -0.000001 -0.000036 -0.000068 0.000067 0.000001 0.015357

33 H 0.000000 -0.000000 0.000008 0.000002 0.000000 -0.000020

34 H 0.000000 0.000000 -0.000000 -0.000000 0.000001 -0.000000

35 H 0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000000

36 H 0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000000

37 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

38 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

39 H 0.000000 0.000000 0.000000 -0.000000 0.000000 0.000000

40 H -0.046224 -0.000824 -0.000062 0.000450 -0.004376 0.000010

41 H -0.046224 -0.000824 -0.000062 0.000450 -0.004376 0.000010

42 H -0.042159 -0.005079 0.000194 -0.000251 0.005952 -0.000010

43 H -0.000000 -0.000021 0.000102 0.000012 -0.000000 0.004586

44 H -0.000000 -0.000021 0.000102 0.000012 -0.000000 0.004586

45 H 0.000000 -0.000001 0.000044 0.000000 0.000000 0.000108

19 20 21 22 23 24

1 C 0.000155 -0.000051 -0.000000 -0.000000 -0.000004 -0.000001

2 N -0.002911 0.000207 0.000002 0.000003 0.000155 -0.000006

3 C 0.000207 -0.000011 -0.000000 -0.000000 -0.000051 -0.000031

4 C 0.000002 -0.000000 0.000000 -0.000000 -0.000000 -0.000000

5 C 0.000003 -0.000000 -0.000000 0.000000 -0.000000 -0.000000

6 N -0.000006 -0.000001 -0.000000 -0.000000 -0.000024 -0.000158

7 C 0.000424 -0.000009 -0.000003 0.000019 -0.001021 -0.001780

8 N -0.021985 0.000088 -0.000080 0.000436 -0.002309 -0.090268

9 C -0.003089 -0.000468 0.000126 0.003211 -0.107307 0.602625

10 C -0.000153 0.000019 0.000020 -0.000462 0.004619 -0.079130

11 C -0.000189 -0.000003 0.000000 0.000010 -0.000306 0.004811

12 N -0.000006 -0.000031 -0.000000 -0.000000 -0.000001 0.000000

13 C -0.000065 0.000135 0.000021 0.000000 -0.000003 -0.000000

14 C 0.000209 0.004346 -0.000400 0.000011 0.000018 -0.000000

15 C -0.001764 -0.106474 0.002323 -0.000413 -0.000603 -0.000016

16 N -0.022050 -0.003182 -0.000001 -0.000199 0.000278 -0.000004

17 C 0.000255 -0.000823 0.000015 -0.000003 -0.000009 -0.000001

18 N -0.080224 0.519635 -0.081750 0.005776 -0.001269 -0.000145

19 N 7.100454 0.383096 -0.068571 -0.102550 0.411127 -0.073130

20 C 0.383096 4.730770 0.472944 -0.076483 -0.145344 0.000941

21 C -0.068571 0.472944 5.089463 0.578888 -0.062046 0.004487

22 C -0.102550 -0.076483 0.578888 5.194834 0.465269 -0.047541

23 C 0.411127 -0.145344 -0.062046 0.465269 4.700520 0.474403

24 N -0.073130 0.000941 0.004487 -0.047541 0.474403 6.615620

25 Zn 0.129604 -0.017915 -0.000562 0.000330 -0.016385 -0.005796

26 C -0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000000

27 H 0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000

28 C 0.000066 0.000000 -0.000001 -0.000026 -0.000446 0.016158

29 H 0.000001 0.000000 0.000000 -0.000000 0.000013 -0.000004

30 C 0.000001 0.000002 -0.000000 0.000000 0.000000 -0.000000

31 H 0.000083 -0.000115 -0.000180 -0.000006 0.000002 0.000000

32 C 0.009919 -0.073690 0.260459 -0.060338 0.010329 -0.000026

33 H 0.007376 0.010489 -0.047350 0.396831 -0.053905 0.006950

34 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

35 H 0.000000 0.000000 0.000000 -0.000000 0.000000 0.000000

36 H 0.000000 0.000000 0.000000 -0.000000 0.000000 0.000000

37 H 0.000015 -0.000000 0.000000 -0.000020 -0.000051 0.004897

38 H 0.000015 -0.000000 0.000000 -0.000020 -0.000051 0.004897

39 H 0.000000 0.000000 0.000000 -0.000001 0.000043 0.000119

40 H 0.000000 -0.000000 0.000000 -0.000000 0.000000 -0.000000

41 H 0.000000 -0.000000 0.000000 -0.000000 0.000000 -0.000000

42 H -0.000000 0.000001 0.000000 0.000000 -0.000000 -0.000000

43 H 0.000437 -0.005916 -0.047126 0.000101 -0.000018 0.000007

44 H 0.000437 -0.005916 -0.047126 0.000101 -0.000018 0.000007

45 H -0.000244 0.006085 -0.043360 -0.005191 0.000222 -0.000012

25 26 27 28 29 30

1 C -0.016385 0.010329 -0.053905 0.000000 0.000002 -0.000446

2 N 0.129604 0.009919 0.007376 0.000001 0.000083 0.000066

3 C -0.017915 -0.073690 0.010489 0.000002 -0.000115 0.000000

4 C -0.000562 0.260459 -0.047350 -0.000000 -0.000180 -0.000001

5 C 0.000330 -0.060338 0.396831 0.000000 -0.000006 -0.000026

6 N -0.005669 0.015357 -0.000020 -0.000019 0.007631 0.000000

7 C -0.016828 -0.000068 0.000008 0.010558 -0.050383 0.000000

8 N 0.127782 0.000067 0.000002 0.009879 0.006871 -0.000000

9 C -0.018407 0.000001 0.000000 -0.068459 0.010448 0.000000

10 C -0.000267 -0.000001 0.000000 0.256587 -0.046241 -0.000000

11 C 0.000203 -0.000036 -0.000000 -0.060337 0.394013 -0.000000

12 N -0.005796 -0.000026 0.006950 -0.000000 0.000000 0.016158

13 C -0.000267 -0.000000 -0.000181 -0.000000 -0.000000 0.256587

14 C 0.000203 0.000000 -0.000006 -0.000000 -0.000000 -0.060337

15 C -0.016828 0.000000 0.000002 0.000000 0.000000 0.010558

16 N 0.127782 0.000001 0.000087 -0.000000 0.000000 0.009879

17 C -0.018407 -0.000000 0.000079 0.000000 -0.000000 -0.068459

18 N -0.005669 -0.000000 0.000000 0.000000 -0.000000 -0.000019

19 N 0.129604 -0.000000 0.000000 0.000066 0.000001 0.000001

20 C -0.017915 0.000000 -0.000000 0.000000 0.000000 0.000002

21 C -0.000562 -0.000000 -0.000000 -0.000001 0.000000 -0.000000

22 C 0.000330 -0.000000 -0.000000 -0.000026 -0.000000 0.000000

23 C -0.016385 0.000000 -0.000000 -0.000446 0.000013 0.000000

24 N -0.005796 0.000000 -0.000000 0.016158 -0.000004 -0.000000

25 Zn 10.253241 0.000330 -0.000137 0.000360 -0.000085 0.000360

26 C 0.000330 5.384505 -0.004614 -0.000000 0.000085 -0.000000

27 H -0.000137 -0.004614 0.483323 -0.000000 -0.000000 0.000084

28 C 0.000360 -0.000000 -0.000000 5.380172 -0.005155 0.000000

29 H -0.000085 0.000085 -0.000000 -0.005155 0.468439 -0.000000

30 C 0.000360 -0.000000 0.000084 0.000000 -0.000000 5.380172

31 H -0.000085 -0.000000 -0.000000 -0.000000 0.000000 -0.005155

32 C 0.000330 0.000000 -0.000000 -0.000000 -0.000000 -0.000000

33 H -0.000137 -0.000000 0.000000 0.000084 -0.000000 -0.000000

34 H 0.000088 0.390271 0.001621 -0.000000 0.000001 -0.000000

35 H 0.000080 0.390239 -0.000153 -0.000000 0.000046 0.000000

36 H 0.000080 0.390239 -0.000153 -0.000000 0.000046 0.000000

37 H 0.000077 0.000000 0.000000 0.389535 -0.000144 0.000000

38 H 0.000077 0.000000 0.000000 0.389535 -0.000144 0.000000

39 H 0.000089 -0.000000 0.000000 0.389645 0.001403 0.000000

40 H 0.000077 -0.000000 0.000048 0.000000 -0.000000 0.389535

41 H 0.000077 -0.000000 0.000048 0.000000 -0.000000 0.389535

42 H 0.000089 -0.000000 0.000001 0.000000 -0.000000 0.389645

43 H 0.000080 0.000000 -0.000000 0.000000 0.000000 -0.000000

44 H 0.000080 0.000000 -0.000000 0.000000 0.000000 -0.000000

45 H 0.000088 -0.000000 -0.000000 -0.000000 0.000000 -0.000000

31 32 33 34 35 36

1 C 0.000013 0.000000 -0.000000 0.000222 -0.000018 -0.000018

2 N 0.000001 -0.000000 0.000000 -0.000244 0.000437 0.000437

3 C 0.000000 0.000000 -0.000000 0.006085 -0.005916 -0.005916

4 C 0.000000 -0.000000 -0.000000 -0.043360 -0.047126 -0.047126

5 C -0.000000 -0.000000 -0.000000 -0.005191 0.000101 0.000101

6 N -0.000000 -0.000000 0.000000 0.000108 0.004586 0.004586

7 C 0.000000 0.000000 0.000002 0.000044 0.000102 0.000102

8 N 0.000000 0.000001 0.000087 0.000000 0.000012 0.000012

9 C -0.000000 -0.000000 0.000079 0.000000 -0.000000 -0.000000

10 C -0.000000 -0.000000 -0.000181 0.000000 -0.000000 -0.000000

11 C -0.000000 0.000000 -0.000006 -0.000001 -0.000021 -0.000021

12 N -0.000004 0.000000 -0.000000 -0.000012 0.000007 0.000007

13 C -0.046241 -0.000001 0.000000 0.000000 0.000000 0.000000

14 C 0.394013 -0.000036 -0.000000 0.000000 -0.000000 -0.000000

15 C -0.050383 -0.000068 0.000008 -0.000000 0.000000 0.000000

16 N 0.006871 0.000067 0.000002 -0.000000 0.000000 0.000000

17 C 0.010448 0.000001 0.000000 0.000001 -0.000000 -0.000000

18 N 0.007631 0.015357 -0.000020 -0.000000 -0.000000 -0.000000

19 N 0.000083 0.009919 0.007376 0.000000 0.000000 0.000000

20 C -0.000115 -0.073690 0.010489 0.000000 0.000000 0.000000

21 C -0.000180 0.260459 -0.047350 0.000000 0.000000 0.000000

22 C -0.000006 -0.060338 0.396831 0.000000 -0.000000 -0.000000

23 C 0.000002 0.010329 -0.053905 0.000000 0.000000 0.000000

24 N 0.000000 -0.000026 0.006950 0.000000 0.000000 0.000000

25 Zn -0.000085 0.000330 -0.000137 0.000088 0.000080 0.000080

26 C -0.000000 0.000000 -0.000000 0.390271 0.390239 0.390239

27 H -0.000000 -0.000000 0.000000 0.001621 -0.000153 -0.000153

28 C -0.000000 -0.000000 0.000084 -0.000000 -0.000000 -0.000000

29 H 0.000000 -0.000000 -0.000000 0.000001 0.000046 0.000046

30 C -0.005155 -0.000000 -0.000000 -0.000000 0.000000 0.000000

31 H 0.468439 0.000085 -0.000000 0.000000 0.000000 0.000000

32 C 0.000085 5.384505 -0.004614 -0.000000 0.000000 0.000000

33 H -0.000000 -0.004614 0.483323 -0.000000 -0.000000 -0.000000

34 H 0.000000 -0.000000 -0.000000 0.477218 -0.027946 -0.027946

35 H 0.000000 0.000000 -0.000000 -0.027946 0.496215 -0.034980

36 H 0.000000 0.000000 -0.000000 -0.027946 -0.034980 0.496215

37 H -0.000000 -0.000000 0.000048 0.000000 0.000000 -0.000000

38 H -0.000000 -0.000000 0.000048 0.000000 -0.000000 0.000000

39 H -0.000000 -0.000000 0.000001 -0.000000 -0.000000 -0.000000

40 H -0.000144 0.000000 0.000000 -0.000000 -0.000000 0.000000

41 H -0.000144 0.000000 0.000000 -0.000000 0.000000 -0.000000

42 H 0.001403 -0.000000 0.000000 -0.000000 0.000000 0.000000

43 H 0.000046 0.390239 -0.000153 0.000000 -0.000000 0.000000

44 H 0.000046 0.390239 -0.000153 0.000000 0.000000 -0.000000

45 H 0.000001 0.390271 0.001621 0.000000 0.000000 0.000000

37 38 39 40 41 42

1 C 0.000000 0.000000 -0.000000 -0.000051 -0.000051 0.000043

2 N 0.000000 0.000000 -0.000000 0.000015 0.000015 0.000000

3 C -0.000000 -0.000000 0.000001 -0.000000 -0.000000 0.000000

4 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

5 C -0.000000 -0.000000 0.000000 -0.000020 -0.000020 -0.000001

6 N 0.000010 0.000010 -0.000010 0.000000 0.000000 0.000000

7 C -0.000062 -0.000062 0.000194 0.000000 0.000000 0.000000

8 N 0.000450 0.000450 -0.000251 0.000000 0.000000 -0.000000

9 C -0.004376 -0.004376 0.005952 0.000000 0.000000 0.000000

10 C -0.046224 -0.046224 -0.042159 0.000000 0.000000 0.000000

11 C -0.000824 -0.000824 -0.005079 0.000000 0.000000 0.000000

12 N -0.000000 -0.000000 -0.000000 0.004897 0.004897 0.000119

13 C 0.000000 0.000000 0.000000 -0.046224 -0.046224 -0.042159

14 C 0.000000 0.000000 0.000000 -0.000824 -0.000824 -0.005079

15 C 0.000000 0.000000 0.000000 -0.000062 -0.000062 0.000194

16 N 0.000000 0.000000 -0.000000 0.000450 0.000450 -0.000251

17 C 0.000000 0.000000 0.000000 -0.004376 -0.004376 0.005952

18 N 0.000000 0.000000 0.000000 0.000010 0.000010 -0.000010

19 N 0.000015 0.000015 0.000000 0.000000 0.000000 -0.000000

20 C -0.000000 -0.000000 0.000000 -0.000000 -0.000000 0.000001

21 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

22 C -0.000020 -0.000020 -0.000001 -0.000000 -0.000000 0.000000

23 C -0.000051 -0.000051 0.000043 0.000000 0.000000 -0.000000

24 N 0.004897 0.004897 0.000119 -0.000000 -0.000000 -0.000000

25 Zn 0.000077 0.000077 0.000089 0.000077 0.000077 0.000089

26 C 0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000000

27 H 0.000000 0.000000 0.000000 0.000048 0.000048 0.000001

28 C 0.389535 0.389535 0.389645 0.000000 0.000000 0.000000

29 H -0.000144 -0.000144 0.001403 -0.000000 -0.000000 -0.000000

30 C 0.000000 0.000000 0.000000 0.389535 0.389535 0.389645

31 H -0.000000 -0.000000 -0.000000 -0.000144 -0.000144 0.001403

32 C -0.000000 -0.000000 -0.000000 0.000000 0.000000 -0.000000

33 H 0.000048 0.000048 0.000001 0.000000 0.000000 0.000000

34 H 0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000000

35 H 0.000000 -0.000000 -0.000000 -0.000000 0.000000 0.000000

36 H -0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000000

37 H 0.482498 -0.031928 -0.026543 0.000000 -0.000000 0.000000

38 H -0.031928 0.482498 -0.026543 -0.000000 0.000000 0.000000

39 H -0.026543 -0.026543 0.468563 0.000000 0.000000 0.000000

40 H 0.000000 -0.000000 0.000000 0.482498 -0.031928 -0.026543

41 H -0.000000 0.000000 0.000000 -0.031928 0.482498 -0.026543

42 H 0.000000 0.000000 0.000000 -0.026543 -0.026543 0.468563

43 H -0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000000

44 H 0.000000 -0.000000 0.000000 -0.000000 0.000000 -0.000000

45 H -0.000000 -0.000000 -0.000000 0.000000 0.000000 -0.000000

43 44 45

1 C 0.000000 0.000000 0.000000

2 N 0.000000 0.000000 0.000000

3 C 0.000000 0.000000 0.000000

4 C 0.000000 0.000000 0.000000

5 C -0.000000 -0.000000 0.000000

6 N -0.000000 -0.000000 -0.000000

7 C 0.000000 0.000000 -0.000000

8 N 0.000000 0.000000 -0.000000

9 C -0.000000 -0.000000 0.000001

10 C 0.000000 0.000000 0.000000

11 C -0.000000 -0.000000 0.000000

12 N 0.000000 0.000000 0.000000

13 C -0.000000 -0.000000 0.000000

14 C -0.000021 -0.000021 -0.000001

15 C 0.000102 0.000102 0.000044

16 N 0.000012 0.000012 0.000000

17 C -0.000000 -0.000000 0.000000

18 N 0.004586 0.004586 0.000108

19 N 0.000437 0.000437 -0.000244

20 C -0.005916 -0.005916 0.006085

21 C -0.047126 -0.047126 -0.043360

22 C 0.000101 0.000101 -0.005191

23 C -0.000018 -0.000018 0.000222

24 N 0.000007 0.000007 -0.000012

25 Zn 0.000080 0.000080 0.000088

26 C 0.000000 0.000000 -0.000000

27 H -0.000000 -0.000000 -0.000000

28 C 0.000000 0.000000 -0.000000

29 H 0.000000 0.000000 0.000000

30 C -0.000000 -0.000000 -0.000000

31 H 0.000046 0.000046 0.000001

32 C 0.390239 0.390239 0.390271

33 H -0.000153 -0.000153 0.001621

34 H 0.000000 0.000000 0.000000

35 H -0.000000 0.000000 0.000000

36 H 0.000000 -0.000000 0.000000

37 H -0.000000 0.000000 -0.000000

38 H 0.000000 -0.000000 -0.000000

39 H 0.000000 0.000000 -0.000000

40 H 0.000000 -0.000000 0.000000

41 H -0.000000 0.000000 0.000000

42 H -0.000000 -0.000000 -0.000000

43 H 0.496215 -0.034980 -0.027946

44 H -0.034980 0.496215 -0.027946

45 H -0.027946 -0.027946 0.477218

Atomic-Atomic Spin Densities.

1 2 3 4 5 6

1 C 0.137535 0.004336 -0.011796 -0.015064 0.037674 0.000799

2 N 0.004336 -0.039374 0.001166 -0.001776 -0.000709 0.000979

3 C -0.011796 0.001166 0.144097 0.041631 -0.013188 -0.039136

4 C -0.015064 -0.001776 0.041631 0.108609 -0.037620 -0.005676

5 C 0.037674 -0.000709 -0.013188 -0.037620 0.071336 0.000452

6 N 0.000799 0.000979 -0.039136 -0.005676 0.000452 0.089722

7 C 0.000077 0.000146 -0.004845 -0.000418 0.000044 0.021727

8 N -0.000131 -0.000072 0.002445 0.000066 -0.000012 -0.003711

9 C 0.000004 0.000010 -0.000121 -0.000002 0.000000 0.000214

10 C -0.000000 -0.000000 0.000030 -0.000000 -0.000000 -0.000332

11 C -0.000003 -0.000004 0.000258 0.000029 -0.000000 -0.001184

12 N -0.037909 0.000428 0.000769 0.000564 -0.005057 -0.000003

13 C 0.000339 -0.000000 -0.000003 -0.000000 0.000027 0.000000

14 C 0.000035 0.000001 0.000000 -0.000000 -0.000000 0.000000

15 C -0.000120 -0.000000 0.000004 0.000000 -0.000002 -0.000000

16 N 0.002335 0.000087 -0.000142 -0.000012 0.000058 0.000003

17 C -0.004593 0.000031 0.000075 0.000041 -0.000379 -0.000002

18 N -0.000003 -0.000000 0.000000 0.000000 -0.000000 -0.000000

19 N 0.000000 -0.000013 0.000002 0.000000 -0.000000 -0.000000

20 C 0.000006 0.000002 -0.000002 -0.000000 0.000000 0.000000

21 C 0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000000

22 C -0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000000

23 C -0.000002 0.000000 0.000006 0.000000 -0.000000 -0.000003

24 N 0.000000 0.000000 -0.000003 -0.000000 0.000000 0.000006

25 Zn 0.000053 0.000294 0.000069 -0.000082 -0.000074 0.000162

26 C -0.000178 -0.000001 -0.000845 -0.003432 0.001864 0.000317

27 H 0.000159 -0.000035 -0.000199 0.000254 0.000346 -0.000001

28 C -0.000000 0.000000 0.000000 -0.000000 -0.000000 -0.000000

29 H -0.000000 -0.000000 -0.000013 0.000003 0.000000 0.000027

30 C -0.000017 -0.000000 -0.000000 0.000000 0.000002 0.000000

31 H 0.000000 0.000000 0.000000 -0.000000 -0.000000 0.000000

32 C -0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000000

33 H 0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.000000

34 H 0.000005 -0.000001 0.000024 -0.000238 0.000010 -0.000004

35 H 0.000063 0.000006 -0.000975 -0.002705 0.000468 0.000345

36 H 0.000063 0.000006 -0.000975 -0.002705 0.000468 0.000345

37 H 0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000001

38 H 0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000001

39 H 0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000000

40 H -0.000057 -0.000000 0.000000 0.000000 -0.000008 -0.000000

41 H -0.000057 -0.000000 0.000000 0.000000 -0.000008 -0.000000

42 H -0.000000 -0.000000 -0.000000 0.000000 -0.000000 -0.000000

43 H -0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000000

44 H -0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000000

45 H 0.000000 -0.000000 -0.000000 -0.000000 0.000000 0.000000

7 8 9 10 11 12

1 C 0.000077 -0.000131 0.000004 -0.000000 -0.000003 -0.037909

2 N 0.000146 -0.000072 0.000010 -0.000000 -0.000004 0.000428

3 C -0.004845 0.002445 -0.000121 0.000030 0.000258 0.000769

4 C -0.000418 0.000066 -0.000002 -0.000000 0.000029 0.000564

5 C 0.000044 -0.000012 0.000000 -0.000000 -0.000000 -0.005057

6 N 0.021727 -0.003711 0.000214 -0.000332 -0.001184 -0.000003

7 C -0.014623 -0.015549 0.003761 0.001155 -0.006806 -0.000002

8 N -0.015549 0.108121 -0.014017 0.002298 0.002384 0.000003

9 C 0.003761 -0.014017 -0.018519 -0.007792 0.000946 -0.000000

10 C 0.001155 0.002298 -0.007792 -0.007236 0.007696 0.000000

11 C -0.006806 0.002384 0.000946 0.007696 -0.006296 0.000000

12 N -0.000002 0.000003 -0.000000 0.000000 0.000000 0.092169

13 C 0.000000 -0.000000 0.000000 -0.000000 -0.000000 -0.001112

14 C 0.000000 -0.000000 0.000000 -0.000000 -0.000000 -0.000363

15 C -0.000001 0.000006 -0.000001 0.000000 0.000000 0.000256

16 N 0.000006 -0.000062 0.000005 -0.000000 -0.000000 -0.003651

17 C -0.000001 0.000005 -0.000001 0.000000 0.000000 0.021014

18 N -0.000000 0.000003 -0.000002 0.000000 0.000000 0.000006

19 N -0.000000 0.000087 0.000031 -0.000000 0.000001 0.000000

20 C 0.000004 -0.000142 0.000075 -0.000003 0.000000 -0.000003

21 C 0.000000 -0.000012 0.000041 -0.000000 -0.000000 -0.000000

22 C -0.000002 0.000058 -0.000379 0.000027 -0.000000 0.000000

23 C -0.000120 0.002335 -0.004593 0.000339 0.000035 0.000000

24 N 0.000256 -0.003651 0.021014 -0.001112 -0.000363 -0.000000

25 Zn -0.000029 -0.001922 0.000084 0.000012 0.000017 0.000131

26 C 0.000019 -0.000000 0.000000 -0.000000 -0.000003 -0.000001

27 H -0.000000 -0.000000 -0.000000 -0.000000 0.000000 -0.000026

28 C -0.000041 0.000007 0.000218 0.001178 -0.000127 0.000000

29 H 0.000123 -0.000008 0.000001 -0.000063 -0.000015 -0.000000

30 C -0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000126

31 H 0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000001

32 C -0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000000

33 H 0.000000 0.000000 -0.000009 -0.000001 0.000000 0.000000

34 H -0.000000 -0.000000 0.000000 -0.000000 0.000000 -0.000000

35 H 0.000036 -0.000002 0.000000 -0.000000 -0.000004 -0.000001

36 H 0.000036 -0.000002 0.000000 -0.000000 -0.000004 -0.000001

37 H 0.000010 -0.000039 0.000309 -0.000064 -0.000114 -0.000000

38 H 0.000010 -0.000039 0.000309 -0.000064 -0.000114 -0.000000

39 H 0.000000 -0.000000 -0.000001 0.000060 -0.000003 0.000000

40 H -0.000000 0.000000 -0.000000 0.000000 0.000000 0.000203

41 H -0.000000 0.000000 -0.000000 0.000000 0.000000 0.000203

42 H -0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000004

43 H -0.000000 0.000000 -0.000000 0.000000 0.000000 0.000000

44 H -0.000000 0.000000 -0.000000 0.000000 0.000000 0.000000

45 H -0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.000000

13 14 15 16 17 18

1 C 0.000339 0.000035 -0.000120 0.002335 -0.004593 -0.000003

2 N -0.000000 0.000001 -0.000000 0.000087 0.000031 -0.000000

3 C -0.000003 0.000000 0.000004 -0.000142 0.000075 0.000000

4 C -0.000000 -0.000000 0.000000 -0.000012 0.000041 0.000000

5 C 0.000027 -0.000000 -0.000002 0.000058 -0.000379 -0.000000

6 N 0.000000 0.000000 -0.000000 0.000003 -0.000002 -0.000000

7 C 0.000000 0.000000 -0.000001 0.000006 -0.000001 -0.000000

8 N -0.000000 -0.000000 0.000006 -0.000062 0.000005 0.000003

9 C 0.000000 0.000000 -0.000001 0.000005 -0.000001 -0.000002

10 C -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

11 C -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

12 N -0.001112 -0.000363 0.000256 -0.003651 0.021014 0.000006

13 C -0.007236 0.007696 0.001155 0.002298 -0.007792 -0.000332

14 C 0.007696 -0.006296 -0.006806 0.002384 0.000946 -0.001184

15 C 0.001155 -0.006806 -0.014623 -0.015549 0.003761 0.021727

16 N 0.002298 0.002384 -0.015549 0.108121 -0.014017 -0.003711

17 C -0.007792 0.000946 0.003761 -0.014017 -0.018519 0.000214

18 N -0.000332 -0.001184 0.021727 -0.003711 0.000214 0.089722

19 N -0.000000 -0.000004 0.000146 -0.000072 0.000010 0.000979

20 C 0.000030 0.000258 -0.004845 0.002445 -0.000121 -0.039136

21 C -0.000000 0.000029 -0.000418 0.000066 -0.000002 -0.005676

22 C -0.000000 -0.000000 0.000044 -0.000012 0.000000 0.000452

23 C -0.000000 -0.000003 0.000077 -0.000131 0.000004 0.000799

24 N 0.000000 0.000000 -0.000002 0.000003 -0.000000 -0.000003

25 Zn 0.000012 0.000017 -0.000029 -0.001922 0.000084 0.000162

26 C 0.000000 -0.000000 -0.000000 0.000000 -0.000000 -0.000000

27 H -0.000001 0.000000 0.000000 0.000000 -0.000009 -0.000000

28 C 0.000000 -0.000000 -0.000000 -0.000000 0.000000 0.000000

29 H 0.000000 0.000000 0.000000 -0.000000 0.000000 0.000000

30 C 0.001178 -0.000127 -0.000041 0.000007 0.000218 -0.000000

31 H -0.000063 -0.000015 0.000123 -0.000008 0.000001 0.000027

32 C -0.000000 -0.000003 0.000019 -0.000000 0.000000 0.000317

33 H -0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000001

34 H -0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000000

35 H 0.000000 0.000000 -0.000000 0.000000 -0.000000 -0.000000

36 H 0.000000 0.000000 -0.000000 0.000000 -0.000000 -0.000000

37 H 0.000000 0.000000 -0.000000 0.000000 -0.000000 -0.000000

38 H 0.000000 0.000000 -0.000000 0.000000 -0.000000 -0.000000

39 H -0.000000 -0.000000 -0.000000 0.000000 -0.000000 -0.000000

40 H -0.000064 -0.000114 0.000010 -0.000039 0.000309 0.000001

41 H -0.000064 -0.000114 0.000010 -0.000039 0.000309 0.000001

42 H 0.000060 -0.000003 0.000000 -0.000000 -0.000001 -0.000000

43 H -0.000000 -0.000004 0.000036 -0.000002 0.000000 0.000345

44 H -0.000000 -0.000004 0.000036 -0.000002 0.000000 0.000345

45 H -0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.000004

19 20 21 22 23 24

1 C 0.000000 0.000006 0.000000 -0.000000 -0.000002 0.000000

2 N -0.000013 0.000002 0.000000 -0.000000 0.000000 0.000000

3 C 0.000002 -0.000002 -0.000000 0.000000 0.000006 -0.000003

4 C 0.000000 -0.000000 -0.000000 0.000000 0.000000 -0.000000

5 C -0.000000 0.000000 0.000000 -0.000000 -0.000000 0.000000

6 N -0.000000 0.000000 0.000000 -0.000000 -0.000003 0.000006

7 C -0.000000 0.000004 0.000000 -0.000002 -0.000120 0.000256

8 N 0.000087 -0.000142 -0.000012 0.000058 0.002335 -0.003651

9 C 0.000031 0.000075 0.000041 -0.000379 -0.004593 0.021014

10 C -0.000000 -0.000003 -0.000000 0.000027 0.000339 -0.001112

11 C 0.000001 0.000000 -0.000000 -0.000000 0.000035 -0.000363

12 N 0.000000 -0.000003 -0.000000 0.000000 0.000000 -0.000000

13 C -0.000000 0.000030 -0.000000 -0.000000 -0.000000 0.000000

14 C -0.000004 0.000258 0.000029 -0.000000 -0.000003 0.000000

15 C 0.000146 -0.004845 -0.000418 0.000044 0.000077 -0.000002

16 N -0.000072 0.002445 0.000066 -0.000012 -0.000131 0.000003

17 C 0.000010 -0.000121 -0.000002 0.000000 0.000004 -0.000000

18 N 0.000979 -0.039136 -0.005676 0.000452 0.000799 -0.000003

19 N -0.039374 0.001166 -0.001776 -0.000709 0.004336 0.000428

20 C 0.001166 0.144097 0.041631 -0.013188 -0.011796 0.000769

21 C -0.001776 0.041631 0.108609 -0.037620 -0.015064 0.000564

22 C -0.000709 -0.013188 -0.037620 0.071336 0.037674 -0.005057

23 C 0.004336 -0.011796 -0.015064 0.037674 0.137535 -0.037909

24 N 0.000428 0.000769 0.000564 -0.005057 -0.037909 0.092169

25 Zn 0.000294 0.000069 -0.000082 -0.000074 0.000053 0.000131

26 C 0.000000 0.000000 0.000000 -0.000000 -0.000000 0.000000

27 H 0.000000 -0.000000 -0.000000 0.000000 0.000000 0.000000

28 C -0.000000 -0.000000 0.000000 0.000002 -0.000017 -0.000126

29 H 0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.000001

30 C 0.000000 0.000000 -0.000000 -0.000000 -0.000000 0.000000

31 H -0.000000 -0.000013 0.000003 0.000000 -0.000000 -0.000000

32 C -0.000001 -0.000845 -0.003432 0.001864 -0.000178 -0.000001

33 H -0.000035 -0.000199 0.000254 0.000346 0.000159 -0.000026

34 H -0.000000 -0.000000 -0.000000 0.000000 0.000000 -0.000000

35 H 0.000000 0.000000 0.000000 -0.000000 -0.000000 0.000000

36 H 0.000000 0.000000 0.000000 -0.000000 -0.000000 0.000000

37 H -0.000000 0.000000 0.000000 -0.000008 -0.000057 0.000203

38 H -0.000000 0.000000 0.000000 -0.000008 -0.000057 0.000203

39 H -0.000000 -0.000000 0.000000 -0.000000 -0.000000 -0.000004

40 H 0.000000 -0.000000 -0.000000 0.000000 0.000000 -0.000000

41 H 0.000000 -0.000000 -0.000000 0.000000 0.000000 -0.000000

42 H -0.000000 0.000000 0.000000 -0.000000 0.000000 0.000000

43 H 0.000006 -0.000975 -0.002705 0.000468 0.000063 -0.000001

44 H 0.000006 -0.000975 -0.002705 0.000468 0.000063 -0.000001

45 H -0.000001 0.000024 -0.000238 0.000010 0.000005 -0.000000

25 26 27 28 29 30

1 C 0.000053 -0.000178 0.000159 -0.000000 -0.000000 -0.000017

2 N 0.000294 -0.000001 -0.000035 0.000000 -0.000000 -0.000000

3 C 0.000069 -0.000845 -0.000199 0.000000 -0.000013 -0.000000

4 C -0.000082 -0.003432 0.000254 -0.000000 0.000003 0.000000

5 C -0.000074 0.001864 0.000346 -0.000000 0.000000 0.000002

6 N 0.000162 0.000317 -0.000001 -0.000000 0.000027 0.000000

7 C -0.000029 0.000019 -0.000000 -0.000041 0.000123 -0.000000

8 N -0.001922 -0.000000 -0.000000 0.000007 -0.000008 -0.000000

9 C 0.000084 0.000000 -0.000000 0.000218 0.000001 0.000000

10 C 0.000012 -0.000000 -0.000000 0.001178 -0.000063 0.000000

11 C 0.000017 -0.000003 0.000000 -0.000127 -0.000015 -0.000000

12 N 0.000131 -0.000001 -0.000026 0.000000 -0.000000 -0.000126

13 C 0.000012 0.000000 -0.000001 0.000000 0.000000 0.001178

14 C 0.000017 -0.000000 0.000000 -0.000000 0.000000 -0.000127

15 C -0.000029 -0.000000 0.000000 -0.000000 0.000000 -0.000041

16 N -0.001922 0.000000 0.000000 -0.000000 -0.000000 0.000007

17 C 0.000084 -0.000000 -0.000009 0.000000 0.000000 0.000218

18 N 0.000162 -0.000000 -0.000000 0.000000 0.000000 -0.000000

19 N 0.000294 0.000000 0.000000 -0.000000 0.000000 0.000000

20 C 0.000069 0.000000 -0.000000 -0.000000 0.000000 0.000000

21 C -0.000082 0.000000 -0.000000 0.000000 -0.000000 -0.000000

22 C -0.000074 -0.000000 0.000000 0.000002 -0.000000 -0.000000

23 C 0.000053 -0.000000 0.000000 -0.000017 0.000000 -0.000000

24 N 0.000131 0.000000 0.000000 -0.000126 -0.000001 0.000000

25 Zn -0.000796 -0.000010 0.000001 -0.000006 -0.000002 -0.000006

26 C -0.000010 -0.009801 0.000250 0.000000 -0.000001 0.000000

27 H 0.000001 0.000250 -0.004367 -0.000000 0.000000 -0.000001

28 C -0.000006 0.000000 -0.000000 -0.000004 -0.000012 0.000000

29 H -0.000002 -0.000001 0.000000 -0.000012 0.000150 0.000000

30 C -0.000006 0.000000 -0.000001 0.000000 0.000000 -0.000004

31 H -0.000002 -0.000000 0.000000 0.000000 0.000000 -0.000012

32 C -0.000010 0.000000 -0.000000 0.000000 -0.000000 0.000000

33 H 0.000001 -0.000000 0.000000 -0.000001 0.000000 -0.000000

34 H 0.000001 0.000494 -0.000048 -0.000000 0.000000 0.000000

35 H 0.000000 0.001775 0.000004 -0.000000 -0.000001 0.000000

36 H 0.000000 0.001775 0.000004 -0.000000 -0.000001 0.000000

37 H -0.000001 0.000000 -0.000000 -0.000361 0.000001 0.000000

38 H -0.000001 0.000000 -0.000000 -0.000361 0.000001 0.000000

39 H -0.000001 0.000000 -0.000000 -0.000025 0.000011 -0.000000

40 H -0.000001 -0.000000 -0.000001 0.000000 0.000000 -0.000361

41 H -0.000001 -0.000000 -0.000001 0.000000 0.000000 -0.000361

42 H -0.000001 0.000000 -0.000000 -0.000000 0.000000 -0.000025

43 H 0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000000

44 H 0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000000

45 H 0.000001 -0.000000 0.000000 0.000000 -0.000000 -0.000000

31 32 33 34 35 36

1 C 0.000000 -0.000000 0.000000 0.000005 0.000063 0.000063

2 N 0.000000 0.000000 0.000000 -0.000001 0.000006 0.000006

3 C 0.000000 0.000000 -0.000000 0.000024 -0.000975 -0.000975

4 C -0.000000 0.000000 -0.000000 -0.000238 -0.002705 -0.002705

5 C -0.000000 -0.000000 0.000000 0.000010 0.000468 0.000468

6 N 0.000000 -0.000000 -0.000000 -0.000004 0.000345 0.000345

7 C 0.000000 -0.000000 0.000000 -0.000000 0.000036 0.000036

8 N -0.000000 0.000000 0.000000 -0.000000 -0.000002 -0.000002

9 C 0.000000 -0.000000 -0.000009 0.000000 0.000000 0.000000

10 C 0.000000 0.000000 -0.000001 -0.000000 -0.000000 -0.000000

11 C 0.000000 -0.000000 0.000000 0.000000 -0.000004 -0.000004

12 N -0.000001 0.000000 0.000000 -0.000000 -0.000001 -0.000001

13 C -0.000063 -0.000000 -0.000000 -0.000000 0.000000 0.000000

14 C -0.000015 -0.000003 0.000000 0.000000 0.000000 0.000000

15 C 0.000123 0.000019 -0.000000 -0.000000 -0.000000 -0.000000

16 N -0.000008 -0.000000 -0.000000 0.000000 0.000000 0.000000

17 C 0.000001 0.000000 -0.000000 -0.000000 -0.000000 -0.000000

18 N 0.000027 0.000317 -0.000001 0.000000 -0.000000 -0.000000

19 N -0.000000 -0.000001 -0.000035 -0.000000 0.000000 0.000000

20 C -0.000013 -0.000845 -0.000199 -0.000000 0.000000 0.000000

21 C 0.000003 -0.003432 0.000254 -0.000000 0.000000 0.000000

22 C 0.000000 0.001864 0.000346 0.000000 -0.000000 -0.000000

23 C -0.000000 -0.000178 0.000159 0.000000 -0.000000 -0.000000

24 N -0.000000 -0.000001 -0.000026 -0.000000 0.000000 0.000000

25 Zn -0.000002 -0.000010 0.000001 0.000001 0.000000 0.000000

26 C -0.000000 0.000000 -0.000000 0.000494 0.001775 0.001775

27 H 0.000000 -0.000000 0.000000 -0.000048 0.000004 0.000004

28 C 0.000000 0.000000 -0.000001 -0.000000 -0.000000 -0.000000

29 H 0.000000 -0.000000 0.000000 0.000000 -0.000001 -0.000001

30 C -0.000012 0.000000 -0.000000 0.000000 0.000000 0.000000

31 H 0.000150 -0.000001 0.000000 -0.000000 0.000000 0.000000

32 C -0.000001 -0.009801 0.000250 -0.000000 -0.000000 -0.000000

33 H 0.000000 0.000250 -0.004367 0.000000 0.000000 0.000000

34 H -0.000000 -0.000000 0.000000 -0.000320 -0.000037 -0.000037

35 H 0.000000 -0.000000 0.000000 -0.000037 0.007545 -0.002357

36 H 0.000000 -0.000000 0.000000 -0.000037 -0.002357 0.007545

37 H 0.000000 -0.000000 -0.000001 0.000000 0.000000 -0.000000

38 H 0.000000 -0.000000 -0.000001 0.000000 -0.000000 0.000000

39 H 0.000000 0.000000 -0.000000 0.000000 0.000000 0.000000

40 H 0.000001 0.000000 -0.000000 0.000000 -0.000000 0.000000

41 H 0.000001 0.000000 -0.000000 0.000000 0.000000 -0.000000

42 H 0.000011 0.000000 -0.000000 0.000000 0.000000 0.000000

43 H -0.000001 0.001775 0.000004 -0.000000 -0.000000 0.000000

44 H -0.000001 0.001775 0.000004 -0.000000 0.000000 -0.000000

45 H 0.000000 0.000494 -0.000048 -0.000000 -0.000000 -0.000000

37 38 39 40 41 42

1 C 0.000000 0.000000 0.000000 -0.000057 -0.000057 -0.000000

2 N 0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000000

3 C -0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000000

4 C -0.000000 -0.000000 0.000000 0.000000 0.000000 0.000000

5 C 0.000000 0.000000 -0.000000 -0.000008 -0.000008 -0.000000

6 N 0.000001 0.000001 -0.000000 -0.000000 -0.000000 -0.000000

7 C 0.000010 0.000010 0.000000 -0.000000 -0.000000 -0.000000

8 N -0.000039 -0.000039 -0.000000 0.000000 0.000000 0.000000

9 C 0.000309 0.000309 -0.000001 -0.000000 -0.000000 -0.000000

10 C -0.000064 -0.000064 0.000060 0.000000 0.000000 -0.000000

11 C -0.000114 -0.000114 -0.000003 0.000000 0.000000 -0.000000

12 N -0.000000 -0.000000 0.000000 0.000203 0.000203 -0.000004

13 C 0.000000 0.000000 -0.000000 -0.000064 -0.000064 0.000060

14 C 0.000000 0.000000 -0.000000 -0.000114 -0.000114 -0.000003

15 C -0.000000 -0.000000 -0.000000 0.000010 0.000010 0.000000

16 N 0.000000 0.000000 0.000000 -0.000039 -0.000039 -0.000000

17 C -0.000000 -0.000000 -0.000000 0.000309 0.000309 -0.000001

18 N -0.000000 -0.000000 -0.000000 0.000001 0.000001 -0.000000

19 N -0.000000 -0.000000 -0.000000 0.000000 0.000000 -0.000000

20 C 0.000000 0.000000 -0.000000 -0.000000 -0.000000 0.000000

21 C 0.000000 0.000000 0.000000 -0.000000 -0.000000 0.000000

22 C -0.000008 -0.000008 -0.000000 0.000000 0.000000 -0.000000

23 C -0.000057 -0.000057 -0.000000 0.000000 0.000000 0.000000

24 N 0.000203 0.000203 -0.000004 -0.000000 -0.000000 0.000000

25 Zn -0.000001 -0.000001 -0.000001 -0.000001 -0.000001 -0.000001

26 C 0.000000 0.000000 0.000000 -0.000000 -0.000000 0.000000

27 H -0.000000 -0.000000 -0.000000 -0.000001 -0.000001 -0.000000

28 C -0.000361 -0.000361 -0.000025 0.000000 0.000000 -0.000000

29 H 0.000001 0.000001 0.000011 0.000000 0.000000 0.000000

30 C 0.000000 0.000000 -0.000000 -0.000361 -0.000361 -0.000025

31 H 0.000000 0.000000 0.000000 0.000001 0.000001 0.000011

32 C -0.000000 -0.000000 0.000000 0.000000 0.000000 0.000000

33 H -0.000001 -0.000001 -0.000000 -0.000000 -0.000000 -0.000000

34 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

35 H 0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

36 H -0.000000 0.000000 0.000000 0.000000 -0.000000 0.000000

37 H 0.000489 -0.000414 -0.000007 -0.000000 0.000000 -0.000000

38 H -0.000414 0.000489 -0.000007 0.000000 -0.000000 -0.000000

39 H -0.000007 -0.000007 0.000006 -0.000000 -0.000000 -0.000000

40 H -0.000000 0.000000 -0.000000 0.000489 -0.000414 -0.000007

41 H 0.000000 -0.000000 -0.000000 -0.000414 0.000489 -0.000007

42 H -0.000000 -0.000000 -0.000000 -0.000007 -0.000007 0.000006

43 H -0.000000 0.000000 0.000000 0.000000 -0.000000 0.000000

44 H 0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

45 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

43 44 45

1 C -0.000000 -0.000000 0.000000

2 N 0.000000 0.000000 -0.000000

3 C 0.000000 0.000000 -0.000000

4 C 0.000000 0.000000 -0.000000

5 C -0.000000 -0.000000 0.000000

6 N -0.000000 -0.000000 0.000000

7 C -0.000000 -0.000000 -0.000000

8 N 0.000000 0.000000 0.000000

9 C -0.000000 -0.000000 -0.000000

10 C 0.000000 0.000000 -0.000000

11 C 0.000000 0.000000 0.000000

12 N 0.000000 0.000000 -0.000000

13 C -0.000000 -0.000000 -0.000000

14 C -0.000004 -0.000004 0.000000

15 C 0.000036 0.000036 -0.000000

16 N -0.000002 -0.000002 -0.000000

17 C 0.000000 0.000000 0.000000

18 N 0.000345 0.000345 -0.000004

19 N 0.000006 0.000006 -0.000001

20 C -0.000975 -0.000975 0.000024

21 C -0.002705 -0.002705 -0.000238

22 C 0.000468 0.000468 0.000010

23 C 0.000063 0.000063 0.000005

24 N -0.000001 -0.000001 -0.000000

25 Zn 0.000000 0.000000 0.000001

26 C -0.000000 -0.000000 -0.000000

27 H 0.000000 0.000000 0.000000

28 C 0.000000 0.000000 0.000000

29 H 0.000000 0.000000 -0.000000

30 C -0.000000 -0.000000 -0.000000

31 H -0.000001 -0.000001 0.000000

32 C 0.001775 0.001775 0.000494

33 H 0.000004 0.000004 -0.000048

34 H -0.000000 -0.000000 -0.000000

35 H -0.000000 0.000000 -0.000000

36 H 0.000000 -0.000000 -0.000000

37 H -0.000000 0.000000 0.000000

38 H 0.000000 -0.000000 0.000000

39 H 0.000000 0.000000 0.000000

40 H 0.000000 -0.000000 0.000000

41 H -0.000000 0.000000 0.000000

42 H 0.000000 0.000000 0.000000

43 H 0.007545 -0.002357 -0.000037

44 H -0.002357 0.007545 -0.000037

45 H -0.000037 -0.000037 -0.000320

Mulliken charges and spin densities:

1 2

1 C 0.324175 0.113556

2 N -0.666950 -0.034495

3 C 0.307675 0.118336

4 C -0.010193 0.081468

5 C -0.352566 0.055689

6 N -0.438558 0.065049

7 C 0.358600 -0.015027

8 N -0.695523 0.078446

9 C 0.347988 -0.018413

10 C 0.010877 -0.003874

11 C -0.313349 -0.003674

12 N -0.437870 0.067479

13 C 0.010877 -0.003874

14 C -0.313349 -0.003674

15 C 0.358600 -0.015027

16 N -0.695523 0.078446

17 C 0.347988 -0.018413

18 N -0.438558 0.065049

19 N -0.666950 -0.034495

20 C 0.307675 0.118336

21 C -0.010193 0.081468

22 C -0.352566 0.055689

23 C 0.324175 0.113556

24 N -0.437870 0.067479

25 Zn 1.392662 -0.003403

26 C -0.713028 -0.007777

27 H 0.199570 -0.003672

28 C -0.708137 0.000324

29 H 0.213374 0.000200

30 C -0.708137 0.000324

31 H 0.213374 0.000200

32 C -0.713028 -0.007777

33 H 0.199570 -0.003672

34 H 0.229043 -0.000152

35 H 0.224339 0.004157

36 H 0.224339 0.004157

37 H 0.232642 -0.000052

38 H 0.232642 -0.000052

39 H 0.234579 0.000027

40 H 0.232642 -0.000052

41 H 0.232642 -0.000052

42 H 0.234579 0.000027

43 H 0.224339 0.004157

44 H 0.224339 0.004157

45 H 0.229043 -0.000152

Sum of Mulliken charges = -1.00000 1.00000

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

1 2

1 C 0.324175 0.113556

2 N -0.666950 -0.034495

3 C 0.307675 0.118336

4 C -0.010193 0.081468

5 C -0.152996 0.052017

6 N -0.438558 0.065049

7 C 0.358600 -0.015027

8 N -0.695523 0.078446

9 C 0.347988 -0.018413

10 C 0.010877 -0.003874

11 C -0.099974 -0.003474

12 N -0.437870 0.067479

13 C 0.010877 -0.003874

14 C -0.099974 -0.003474

15 C 0.358600 -0.015027

16 N -0.695523 0.078446

17 C 0.347988 -0.018413

18 N -0.438558 0.065049

19 N -0.666950 -0.034495

20 C 0.307675 0.118336

21 C -0.010193 0.081468

22 C -0.152996 0.052017

23 C 0.324175 0.113556

24 N -0.437870 0.067479

25 Zn 1.392662 -0.003403

26 C -0.035306 0.000385

28 C -0.008275 0.000249

30 C -0.008275 0.000249

32 C -0.035306 0.000385

Electronic spatial extent (au): <R\*\*2>= 11294.4222

Charge= -1.0000 electrons

Dipole moment (field-independent basis, Debye):

X= -0.0000 Y= -0.0000 Z= 0.0000 Tot= 0.0000

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

XX= -209.5998 YY= -189.4382 ZZ= -177.1666

XY= -4.6800 XZ= -0.0000 YZ= 0.0000

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

XX= -17.5316 YY= 2.6300 ZZ= 14.9016

XY= -4.6800 XZ= -0.0000 YZ= 0.0000

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

XXX= 0.0000 YYY= -0.0000 ZZZ= -0.0000 XYY= 0.0000

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

YYZ= -0.0000 XYZ= -0.0000

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

XXXX= -7891.6882 YYYY= -7438.0741 ZZZZ= -217.5587 XXXY= 79.6127

XXXZ= -0.0000 YYYX= -217.4016 YYYZ= 0.0000 ZZZX= -0.0000

ZZZY= -0.0000 XXYY= -2761.3144 XXZZ= -1408.9508 YYZZ= -1393.0171

XXYZ= -0.0000 YYXZ= 0.0000 ZZXY= -5.0579

N-N= 2.760267341802D+03 E-N=-8.600184227058D+03 KE= 1.321005085480D+03

Symmetry AG KE= 6.505256876963D+02

Symmetry BG KE= 6.684521357150D+01

Symmetry AU KE= 2.216795728839D+01

Symmetry BU KE= 5.814662269240D+02

Isotropic Fermi Contact Couplings

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

1 C(13) 0.00381 4.28631 1.52946 1.42976

2 N(14) -0.00813 -2.62573 -0.93693 -0.87585

3 C(13) 0.00347 3.89820 1.39097 1.30030

4 C(13) 0.00047 0.52315 0.18667 0.17450

5 C(13) -0.00246 -2.76153 -0.98538 -0.92115

6 N(14) 0.00571 1.84459 0.65820 0.61529

7 C(13) -0.00439 -4.93684 -1.76159 -1.64675

8 N(14) 0.00863 2.78718 0.99453 0.92970

9 C(13) -0.00465 -5.23000 -1.86619 -1.74454

10 C(13) -0.00047 -0.52707 -0.18807 -0.17581

11 C(13) -0.00037 -0.41569 -0.14833 -0.13866

12 N(14) 0.00638 2.06014 0.73511 0.68719

13 C(13) -0.00047 -0.52707 -0.18807 -0.17581

14 C(13) -0.00037 -0.41569 -0.14833 -0.13866

15 C(13) -0.00439 -4.93684 -1.76159 -1.64675

16 N(14) 0.00863 2.78718 0.99453 0.92970

17 C(13) -0.00465 -5.23000 -1.86619 -1.74454

18 N(14) 0.00571 1.84459 0.65820 0.61529

19 N(14) -0.00813 -2.62573 -0.93693 -0.87585

20 C(13) 0.00347 3.89820 1.39097 1.30030

21 C(13) 0.00047 0.52315 0.18667 0.17450

22 C(13) -0.00246 -2.76153 -0.98538 -0.92115

23 C(13) 0.00381 4.28631 1.52946 1.42976

24 N(14) 0.00638 2.06014 0.73511 0.68719

25 Zn(67) 0.00000 0.00000 0.00000 0.00000

26 C(13) -0.00338 -3.79540 -1.35429 -1.26601

27 H(1) -0.00110 -4.90672 -1.75084 -1.63671

28 C(13) 0.00017 0.19575 0.06985 0.06530

29 H(1) 0.00007 0.29714 0.10603 0.09911

30 C(13) 0.00017 0.19575 0.06985 0.06530

31 H(1) 0.00007 0.29714 0.10603 0.09911

32 C(13) -0.00338 -3.79540 -1.35429 -1.26601

33 H(1) -0.00110 -4.90672 -1.75084 -1.63671

34 H(1) -0.00004 -0.16049 -0.05727 -0.05353

35 H(1) 0.00225 10.07117 3.59364 3.35938

36 H(1) 0.00225 10.07117 3.59364 3.35938

37 H(1) -0.00024 -1.07950 -0.38519 -0.36008

38 H(1) -0.00024 -1.07950 -0.38519 -0.36008

39 H(1) 0.00001 0.03192 0.01139 0.01065

40 H(1) -0.00024 -1.07950 -0.38519 -0.36008

41 H(1) -0.00024 -1.07950 -0.38519 -0.36008

42 H(1) 0.00001 0.03192 0.01139 0.01065

43 H(1) 0.00225 10.07117 3.59364 3.35938

44 H(1) 0.00225 10.07117 3.59364 3.35938

45 H(1) -0.00004 -0.16049 -0.05727 -0.05353

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

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

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

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

1 Atom -0.076377 -0.073275 0.149653

2 Atom 0.026478 0.026779 -0.053256

3 Atom -0.077112 -0.080398 0.157510

4 Atom -0.055628 -0.057907 0.113535

5 Atom -0.036791 -0.038023 0.074814

6 Atom -0.090197 -0.093796 0.183993

7 Atom 0.014127 0.003117 -0.017244

8 Atom -0.086730 -0.092111 0.178841

9 Atom 0.016465 0.005672 -0.022137

10 Atom 0.003442 0.004435 -0.007877

11 Atom 0.002517 0.003229 -0.005746

12 Atom -0.095562 -0.095540 0.191102

13 Atom 0.003442 0.004435 -0.007877

14 Atom 0.002517 0.003229 -0.005746

15 Atom 0.014127 0.003117 -0.017244

16 Atom -0.086730 -0.092111 0.178841

17 Atom 0.016465 0.005672 -0.022137

18 Atom -0.090197 -0.093796 0.183993

19 Atom 0.026478 0.026779 -0.053256

20 Atom -0.077112 -0.080398 0.157510

21 Atom -0.055628 -0.057907 0.113535

22 Atom -0.036791 -0.038023 0.074814

23 Atom -0.076377 -0.073275 0.149653

24 Atom -0.095562 -0.095540 0.191102

25 Atom -0.013747 0.011305 0.002442

26 Atom 0.001519 -0.001214 -0.000305

27 Atom 0.006985 -0.004400 -0.002585

28 Atom -0.000200 0.001455 -0.001255

29 Atom 0.000231 0.000941 -0.001172

30 Atom -0.000200 0.001455 -0.001255

31 Atom 0.000231 0.000941 -0.001172

32 Atom 0.001519 -0.001214 -0.000305

33 Atom 0.006985 -0.004400 -0.002585

34 Atom 0.002489 -0.000879 -0.001610

35 Atom 0.000769 0.000918 -0.001687

36 Atom 0.000769 0.000918 -0.001687

37 Atom -0.000530 0.001329 -0.000799

38 Atom -0.000530 0.001329 -0.000799

39 Atom -0.000184 0.000723 -0.000539

40 Atom -0.000530 0.001329 -0.000799

41 Atom -0.000530 0.001329 -0.000799

42 Atom -0.000184 0.000723 -0.000539

43 Atom 0.000769 0.000918 -0.001687

44 Atom 0.000769 0.000918 -0.001687

45 Atom 0.002489 -0.000879 -0.001610

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

XY XZ YZ

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

1 Atom 0.003335 0.000000 -0.000000

2 Atom 0.000130 0.000000 -0.000000

3 Atom -0.003681 0.000000 0.000000

4 Atom 0.001056 -0.000000 -0.000000

5 Atom -0.000788 -0.000000 0.000000

6 Atom -0.002617 0.000000 0.000000

7 Atom 0.001180 0.000000 -0.000000

8 Atom 0.000938 0.000000 0.000000

9 Atom 0.002246 -0.000000 0.000000

10 Atom 0.000254 -0.000000 -0.000000

11 Atom -0.000640 0.000000 -0.000000

12 Atom 0.002714 -0.000000 0.000000

13 Atom 0.000254 0.000000 -0.000000

14 Atom -0.000640 0.000000 -0.000000

15 Atom 0.001180 -0.000000 0.000000

16 Atom 0.000938 -0.000000 -0.000000

17 Atom 0.002246 -0.000000 0.000000

18 Atom -0.002617 -0.000000 -0.000000

19 Atom 0.000130 -0.000000 0.000000

20 Atom -0.003681 -0.000000 0.000000

21 Atom 0.001056 0.000000 -0.000000

22 Atom -0.000788 -0.000000 -0.000000

23 Atom 0.003335 -0.000000 0.000000

24 Atom 0.002714 0.000000 0.000000

25 Atom -0.005044 0.000000 -0.000000

26 Atom 0.002853 -0.000000 -0.000000

27 Atom -0.004233 -0.000000 0.000000

28 Atom -0.000034 0.000000 -0.000000

29 Atom -0.000777 -0.000000 0.000000

30 Atom -0.000034 -0.000000 -0.000000

31 Atom -0.000777 -0.000000 -0.000000

32 Atom 0.002853 -0.000000 -0.000000

33 Atom -0.004233 -0.000000 -0.000000

34 Atom 0.001464 0.000000 -0.000000

35 Atom 0.002325 -0.000918 -0.001231

36 Atom 0.002325 0.000918 0.001231

37 Atom -0.000361 0.000021 -0.000488

38 Atom -0.000361 -0.000021 0.000488

39 Atom -0.000199 0.000000 -0.000000

40 Atom -0.000361 -0.000021 0.000488

41 Atom -0.000361 0.000021 -0.000488

42 Atom -0.000199 -0.000000 0.000000

43 Atom 0.002325 0.000918 0.001231

44 Atom 0.002325 -0.000918 -0.001231

45 Atom 0.001464 0.000000 -0.000000

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

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Anisotropic Spin Dipole Couplings in Principal Axis System

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

Baa -0.0785 -10.535 -3.759 -3.514 0.8431 -0.5377 0.0000

1 C(13) Bbb -0.0711 -9.547 -3.407 -3.185 0.5377 0.8431 -0.0000

Bcc 0.1497 20.082 7.166 6.699 0.0000 0.0000 1.0000

Baa -0.0533 -2.054 -0.733 -0.685 0.0000 0.0000 1.0000

2 N(14) Bbb 0.0264 1.019 0.364 0.340 0.9369 -0.3496 0.0000

Bcc 0.0268 1.035 0.369 0.345 0.3496 0.9369 -0.0000

Baa -0.0828 -11.109 -3.964 -3.706 0.5443 0.8389 -0.0000

3 C(13) Bbb -0.0747 -10.027 -3.578 -3.345 0.8389 -0.5443 -0.0000

Bcc 0.1575 21.136 7.542 7.050 0.0000 0.0000 1.0000

Baa -0.0583 -7.826 -2.793 -2.611 -0.3652 0.9309 -0.0000

4 C(13) Bbb -0.0552 -7.409 -2.644 -2.471 0.9309 0.3652 0.0000

Bcc 0.1135 15.235 5.436 5.082 0.0000 0.0000 1.0000

Baa -0.0384 -5.154 -1.839 -1.719 0.4382 0.8989 -0.0000

5 C(13) Bbb -0.0364 -4.885 -1.743 -1.630 0.8989 -0.4382 0.0000

Bcc 0.0748 10.039 3.582 3.349 0.0000 0.0000 1.0000

Baa -0.0952 -3.671 -1.310 -1.224 0.4655 0.8850 -0.0000

6 N(14) Bbb -0.0888 -3.426 -1.222 -1.143 0.8850 -0.4655 0.0000

Bcc 0.1840 7.096 2.532 2.367 0.0000 0.0000 1.0000

Baa -0.0172 -2.314 -0.826 -0.772 0.0000 0.0000 1.0000

7 C(13) Bbb 0.0030 0.401 0.143 0.134 -0.1054 0.9944 -0.0000

Bcc 0.0143 1.912 0.682 0.638 0.9944 0.1054 0.0000

Baa -0.0923 -3.559 -1.270 -1.187 -0.1669 0.9860 -0.0000

8 N(14) Bbb -0.0866 -3.339 -1.191 -1.114 0.9860 0.1669 0.0000

Bcc 0.1788 6.898 2.461 2.301 0.0000 0.0000 1.0000

Baa -0.0221 -2.971 -1.060 -0.991 0.0000 0.0000 1.0000

9 C(13) Bbb 0.0052 0.701 0.250 0.234 -0.1959 0.9806 -0.0000

Bcc 0.0169 2.270 0.810 0.757 0.9806 0.1959 0.0000

Baa -0.0079 -1.057 -0.377 -0.353 0.0000 0.0000 1.0000

10 C(13) Bbb 0.0034 0.454 0.162 0.151 0.9722 -0.2340 -0.0000

Bcc 0.0045 0.603 0.215 0.201 0.2340 0.9722 -0.0000

Baa -0.0057 -0.771 -0.275 -0.257 0.0000 0.0000 1.0000

11 C(13) Bbb 0.0021 0.287 0.103 0.096 0.8620 0.5070 0.0000

Bcc 0.0036 0.484 0.173 0.161 -0.5070 0.8620 -0.0000

Baa -0.0983 -3.790 -1.352 -1.264 0.7086 -0.7057 0.0000

12 N(14) Bbb -0.0928 -3.581 -1.278 -1.194 0.7057 0.7086 -0.0000

Bcc 0.1911 7.370 2.630 2.458 0.0000 0.0000 1.0000

Baa -0.0079 -1.057 -0.377 -0.353 0.0000 0.0000 1.0000

13 C(13) Bbb 0.0034 0.454 0.162 0.151 0.9722 -0.2340 0.0000

Bcc 0.0045 0.603 0.215 0.201 0.2340 0.9722 -0.0000

Baa -0.0057 -0.771 -0.275 -0.257 0.0000 0.0000 1.0000

14 C(13) Bbb 0.0021 0.287 0.103 0.096 0.8620 0.5070 0.0000

Bcc 0.0036 0.484 0.173 0.161 -0.5070 0.8620 -0.0000

Baa -0.0172 -2.314 -0.826 -0.772 0.0000 0.0000 1.0000

15 C(13) Bbb 0.0030 0.401 0.143 0.134 -0.1054 0.9944 -0.0000

Bcc 0.0143 1.912 0.682 0.638 0.9944 0.1054 0.0000

Baa -0.0923 -3.559 -1.270 -1.187 -0.1669 0.9860 -0.0000

16 N(14) Bbb -0.0866 -3.339 -1.191 -1.114 0.9860 0.1669 0.0000

Bcc 0.1788 6.898 2.461 2.301 0.0000 0.0000 1.0000

Baa -0.0221 -2.971 -1.060 -0.991 0.0000 0.0000 1.0000

17 C(13) Bbb 0.0052 0.701 0.250 0.234 -0.1959 0.9806 -0.0000

Bcc 0.0169 2.270 0.810 0.757 0.9806 0.1959 0.0000

Baa -0.0952 -3.671 -1.310 -1.224 0.4655 0.8850 -0.0000

18 N(14) Bbb -0.0888 -3.426 -1.222 -1.143 0.8850 -0.4655 -0.0000

Bcc 0.1840 7.096 2.532 2.367 0.0000 0.0000 1.0000

Baa -0.0533 -2.054 -0.733 -0.685 0.0000 0.0000 1.0000

19 N(14) Bbb 0.0264 1.019 0.364 0.340 0.9369 -0.3496 0.0000

Bcc 0.0268 1.035 0.369 0.345 0.3496 0.9369 -0.0000

Baa -0.0828 -11.109 -3.964 -3.706 0.5443 0.8389 -0.0000

20 C(13) Bbb -0.0747 -10.027 -3.578 -3.345 0.8389 -0.5443 0.0000

Bcc 0.1575 21.136 7.542 7.050 0.0000 0.0000 1.0000

Baa -0.0583 -7.826 -2.793 -2.611 -0.3652 0.9309 -0.0000

21 C(13) Bbb -0.0552 -7.409 -2.644 -2.471 0.9309 0.3652 0.0000

Bcc 0.1135 15.235 5.436 5.082 0.0000 0.0000 1.0000

Baa -0.0384 -5.154 -1.839 -1.719 0.4382 0.8989 -0.0000

22 C(13) Bbb -0.0364 -4.885 -1.743 -1.630 0.8989 -0.4382 0.0000

Bcc 0.0748 10.039 3.582 3.349 0.0000 0.0000 1.0000

Baa -0.0785 -10.535 -3.759 -3.514 0.8431 -0.5377 0.0000

23 C(13) Bbb -0.0711 -9.547 -3.407 -3.185 0.5377 0.8431 -0.0000

Bcc 0.1497 20.082 7.166 6.699 0.0000 0.0000 1.0000

Baa -0.0983 -3.790 -1.352 -1.264 0.7086 -0.7057 0.0000

24 N(14) Bbb -0.0928 -3.581 -1.278 -1.194 0.7057 0.7086 0.0000

Bcc 0.1911 7.370 2.630 2.458 0.0000 0.0000 1.0000

Baa -0.0147 -0.493 -0.176 -0.164 0.9817 0.1903 0.0000

25 Zn(67) Bbb 0.0024 0.082 0.029 0.027 0.0000 0.0000 1.0000

Bcc 0.0123 0.411 0.147 0.137 -0.1903 0.9817 0.0000

Baa -0.0030 -0.404 -0.144 -0.135 -0.5329 0.8462 0.0000

26 C(13) Bbb -0.0003 -0.041 -0.015 -0.014 0.0000 0.0000 1.0000

Bcc 0.0033 0.445 0.159 0.148 0.8462 0.5329 -0.0000

Baa -0.0058 -3.095 -1.104 -1.032 0.3143 0.9493 0.0000

27 H(1) Bbb -0.0026 -1.379 -0.492 -0.460 0.0000 0.0000 1.0000

Bcc 0.0084 4.475 1.597 1.493 0.9493 -0.3143 0.0000

Baa -0.0013 -0.168 -0.060 -0.056 0.0000 0.0000 1.0000

28 C(13) Bbb -0.0002 -0.027 -0.010 -0.009 0.9998 0.0203 0.0000

Bcc 0.0015 0.195 0.070 0.065 -0.0203 0.9998 -0.0000

Baa -0.0012 -0.626 -0.223 -0.209 0.0000 0.0000 1.0000

29 H(1) Bbb -0.0003 -0.143 -0.051 -0.048 0.8412 0.5408 -0.0000

Bcc 0.0014 0.769 0.274 0.256 -0.5408 0.8412 -0.0000

Baa -0.0013 -0.168 -0.060 -0.056 0.0000 0.0000 1.0000

30 C(13) Bbb -0.0002 -0.027 -0.010 -0.009 0.9998 0.0203 0.0000

Bcc 0.0015 0.195 0.070 0.065 -0.0203 0.9998 -0.0000

Baa -0.0012 -0.626 -0.223 -0.209 0.0000 0.0000 1.0000

31 H(1) Bbb -0.0003 -0.143 -0.051 -0.048 0.8412 0.5408 -0.0000

Bcc 0.0014 0.769 0.274 0.256 -0.5408 0.8412 0.0000

Baa -0.0030 -0.404 -0.144 -0.135 -0.5329 0.8462 0.0000

32 C(13) Bbb -0.0003 -0.041 -0.015 -0.014 0.0000 -0.0000 1.0000

Bcc 0.0033 0.445 0.159 0.148 0.8462 0.5329 -0.0000

Baa -0.0058 -3.095 -1.104 -1.032 0.3143 0.9493 0.0000

33 H(1) Bbb -0.0026 -1.379 -0.492 -0.460 0.0000 0.0000 1.0000

Bcc 0.0084 4.475 1.597 1.493 0.9493 -0.3143 0.0000

Baa -0.0016 -0.859 -0.307 -0.287 -0.0000 0.0000 1.0000

34 H(1) Bbb -0.0014 -0.761 -0.271 -0.254 -0.3502 0.9367 -0.0000

Bcc 0.0030 1.620 0.578 0.540 0.9367 0.3502 0.0000

Baa -0.0022 -1.161 -0.414 -0.387 -0.0048 0.3727 0.9280

35 H(1) Bbb -0.0014 -0.764 -0.273 -0.255 0.7505 -0.6119 0.2496

Bcc 0.0036 1.925 0.687 0.642 0.6608 0.6977 -0.2767

Baa -0.0022 -1.161 -0.414 -0.387 0.0048 -0.3727 0.9280

36 H(1) Bbb -0.0014 -0.764 -0.273 -0.255 0.7505 -0.6119 -0.2496

Bcc 0.0036 1.925 0.687 0.642 0.6608 0.6977 0.2767

Baa -0.0009 -0.488 -0.174 -0.163 0.1687 0.2352 0.9572

37 H(1) Bbb -0.0006 -0.311 -0.111 -0.104 0.9703 0.1312 -0.2033

Bcc 0.0015 0.800 0.285 0.267 -0.1734 0.9631 -0.2060

Baa -0.0009 -0.488 -0.174 -0.163 -0.1687 -0.2352 0.9572

38 H(1) Bbb -0.0006 -0.311 -0.111 -0.104 0.9703 0.1312 0.2033

Bcc 0.0015 0.800 0.285 0.267 -0.1734 0.9631 0.2060

Baa -0.0005 -0.288 -0.103 -0.096 0.0000 0.0000 1.0000

39 H(1) Bbb -0.0002 -0.120 -0.043 -0.040 0.9787 0.2054 0.0000

Bcc 0.0008 0.408 0.146 0.136 -0.2054 0.9787 -0.0000

Baa -0.0009 -0.488 -0.174 -0.163 -0.1687 -0.2352 0.9572

40 H(1) Bbb -0.0006 -0.311 -0.111 -0.104 0.9703 0.1312 0.2033

Bcc 0.0015 0.800 0.285 0.267 -0.1734 0.9631 0.2060

Baa -0.0009 -0.488 -0.174 -0.163 0.1687 0.2352 0.9572

41 H(1) Bbb -0.0006 -0.311 -0.111 -0.104 0.9703 0.1312 -0.2033

Bcc 0.0015 0.800 0.285 0.267 -0.1734 0.9631 -0.2060

Baa -0.0005 -0.288 -0.103 -0.096 0.0000 0.0000 1.0000

42 H(1) Bbb -0.0002 -0.120 -0.043 -0.040 0.9787 0.2054 -0.0000

Bcc 0.0008 0.408 0.146 0.136 -0.2054 0.9787 -0.0000

Baa -0.0022 -1.161 -0.414 -0.387 0.0048 -0.3727 0.9280

43 H(1) Bbb -0.0014 -0.764 -0.273 -0.255 0.7505 -0.6119 -0.2496

Bcc 0.0036 1.925 0.687 0.642 0.6608 0.6977 0.2767

Baa -0.0022 -1.161 -0.414 -0.387 -0.0048 0.3727 0.9280

44 H(1) Bbb -0.0014 -0.764 -0.273 -0.255 0.7505 -0.6119 0.2496

Bcc 0.0036 1.925 0.687 0.642 0.6608 0.6977 -0.2767

Baa -0.0016 -0.859 -0.307 -0.287 -0.0000 0.0000 1.0000

45 H(1) Bbb -0.0014 -0.761 -0.271 -0.254 -0.3502 0.9367 -0.0000

Bcc 0.0030 1.620 0.578 0.540 0.9367 0.3502 0.0000

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

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Tue Sep 17 14:08:42 2019, MaxMem= 2415919104 cpu: 24.2

(Enter /home/blab/g09/l9999.exe)

1\1\ WCSS.PL-BEM-DHCP-129-94-98-136\FOpt\UB3LYP\GenECP\C20H16N8Zn1(1-,

2)\BLAB\17-Sep-2019\0\\#p opt=GDIIS b3lyp/genecp scrf=(solvent=dmso,sm

d) empiricaldispersion=gd3bj\\ZntAzPanion\\-1,2\C,-2.0749982023,-2.194

7451768,0.\N,-0.7482401247,-1.8687350692,0.\C,-0.0041400404,-3.0160187

197,0.\C,-0.8990576208,-4.1483493165,0.\C,-2.1857447113,-3.6258920937,

0.\N,1.3574381672,-3.1091708982,0.\C,2.1848550387,-2.077015423,0.\N,1.

8631450988,-0.7449845948,0.\C,3.007653027,0.0035184661,0.\C,4.16485495

03,-0.9245923789,0.\C,3.6508847948,-2.1823565709,0.\N,-3.1254795003,-1

.3196675412,0.\C,-4.1648549503,0.9245923789,0.\C,-3.6508847948,2.18235

65709,0.\C,-2.1848550387,2.077015423,0.\N,-1.8631450988,0.7449845948,0

.\C,-3.007653027,-0.0035184661,0.\N,-1.3574381672,3.1091708982,0.\N,0.

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08,4.1483493165,0.\C,2.1857447113,3.6258920937,0.\C,2.0749982023,2.194

7451768,0.\N,3.1254795003,1.3196675412,0.\Zn,0.,0.,0.\C,-0.4784782217,

-5.5829040869,0.\H,-3.1155872738,-4.1800554506,0.\C,5.5881929515,-0.48

34111972,0.\H,4.1956550092,-3.1174540505,0.\C,-5.5881929515,0.48341119

72,0.\H,-4.1956550092,3.1174540505,0.\C,0.4784782217,5.5829040869,0.\H

,3.1155872738,4.1800554506,0.\H,-1.3439265615,-6.2496761425,0.\H,0.130

8411847,-5.8265223596,0.8772041786\H,0.1308411847,-5.8265223596,-0.877

2041786\H,5.8103418993,0.1335758428,0.8767989603\H,5.8103418993,0.1335

758428,-0.8767989603\H,6.2707964913,-1.335503961,0.\H,-5.8103418993,-0

.1335758428,0.8767989603\H,-5.8103418993,-0.1335758428,-0.8767989603\H

,-6.2707964913,1.335503961,0.\H,-0.1308411847,5.8265223596,0.877204178

6\H,-0.1308411847,5.8265223596,-0.8772041786\H,1.3439265615,6.24967614

25,0.\\Version=ES64L-G09RevE.01\State=2-BG\HF=-1276.0158\S2=0.765212\S

2-1=0.\S2A=0.750115\RMSD=7.107e-09\RMSF=8.551e-05\Dipole=0.,0.,0.\Quad

rupole=1.0739489,-12.1529456,11.0789967,-4.9539119,0.,0.\PG=C02H [O(Zn

1),SGH(C20H8N8),X(H8)]\\@

REPARTEE - WHAT YOU THINK OF AFTER YOU BECOME A DEPARTEE.

Job cpu time: 0 days 6 hours 1 minutes 5.5 seconds.

File lengths (MBytes): RWF= 745 Int= 0 D2E= 0 Chk= 34 Scr= 1

Normal termination of Gaussian 09 at Tue Sep 17 14:08:42 2019.