Entering Gaussian System, Link 0=g09

Input=ZntAzP3.com

Output=ZntAzP3.log

Initial command:

/home/blab/g09/l1.exe "/home/blab/g09/scratch/Gau-26621.inp" -scrdir="/home/blab/g09/scratch/"

Entering Link 1 = /home/blab/g09/l1.exe PID= 26628.

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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=ZntAzP3.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 13:48:07 2019, MaxMem= 2415919104 cpu: 1.4

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

-------

ZntAzP3

-------

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3

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 13:48:07 2019, MaxMem= 2415919104 cpu: 6.7

(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 13:48:07 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(3)

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 13:48:07 2019, MaxMem= 2415919104 cpu: 0.4

(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\*

\*\*\*\*

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

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 101 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 13:48:08 2019, MaxMem= 2415919104 cpu: 3.8

(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 13:48:09 2019, MaxMem= 2415919104 cpu: 16.1

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 13:48:09 2019, MaxMem= 2415919104 cpu: 1.7

(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= -1276.13767392719

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>= 1.0000 <S\*\*2>= 2.0000 S= 1.0000

Leave Link 401 at Tue Sep 17 13:48:10 2019, MaxMem= 2415919104 cpu: 21.4

(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 8.88D-15 for 3557.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.78D-15 for 3555 2667.

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

Iteration 1 A^-1\*A deviation from orthogonality is 2.32D-12 for 2196 2167.

E= -1275.11874027699

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

NSaved= 1 IEnMin= 1 EnMin= -1275.11874027699 IErMin= 1 ErrMin= 9.03D-02

ErrMax= 9.03D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.08D+00 BMatP= 4.08D+00

IDIUse=3 WtCom= 9.65D-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= 0.022 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=2.91D-03 MaxDP=1.28D-01 OVMax= 2.05D-01

Cycle 2 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 3.62D-04 CP: 9.95D-01

E= -1275.27145509059 Delta-E= -0.152714813592 Rises=F Damp=T

DIIS: error= 6.01D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.27145509059 IErMin= 2 ErrMin= 6.01D-02

ErrMax= 6.01D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.20D+00 BMatP= 4.08D+00

IDIUse=3 WtCom= 3.99D-01 WtEn= 6.01D-01

Coeff-Com: -0.249D+01 0.349D+01

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

Coeff: -0.995D+00 0.200D+01

Gap= 0.028 Goal= None Shift= 0.000

Gap= 0.048 Goal= None Shift= 0.000

RMSDP=1.61D-03 MaxDP=8.02D-02 DE=-1.53D-01 OVMax= 1.26D-01

Cycle 3 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 1.10D-03 CP: 9.81D-01 3.00D+00

E= -1275.69226756511 Delta-E= -0.420812474521 Rises=F Damp=F

DIIS: error= 2.55D-02 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1275.69226756511 IErMin= 3 ErrMin= 2.55D-02

ErrMax= 2.55D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.70D-01 BMatP= 2.20D+00

IDIUse=3 WtCom= 7.45D-01 WtEn= 2.55D-01

EnCoef did 100 forward-backward iterations

Coeff-Com: -0.141D+00 0.522D+00 0.619D+00

Coeff-En: 0.102D+00 0.170D-02 0.897D+00

Coeff: -0.791D-01 0.390D+00 0.689D+00

Gap= 0.033 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=8.10D-04 MaxDP=4.24D-02 DE=-4.21D-01 OVMax= 6.90D-02

Cycle 4 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 4.76D-04 CP: 9.87D-01 2.93D+00 4.28D-01

E= -1275.81965774304 Delta-E= -0.127390177934 Rises=F Damp=F

DIIS: error= 7.34D-03 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.81965774304 IErMin= 4 ErrMin= 7.34D-03

ErrMax= 7.34D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.60D-02 BMatP= 6.70D-01

IDIUse=3 WtCom= 9.27D-01 WtEn= 7.34D-02

Coeff-Com: 0.125D+00-0.531D-01 0.368D+00 0.561D+00

Coeff-En: 0.000D+00 0.000D+00 0.338D-01 0.966D+00

Coeff: 0.116D+00-0.492D-01 0.343D+00 0.591D+00

Gap= 0.032 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=2.39D-04 MaxDP=1.13D-02 DE=-1.27D-01 OVMax= 4.42D-02

Cycle 5 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 1.40D-04 CP: 9.86D-01 3.00D+00 5.39D-01 7.31D-01

E= -1275.83715664762 Delta-E= -0.017498904577 Rises=F Damp=F

DIIS: error= 3.14D-03 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.83715664762 IErMin= 5 ErrMin= 3.14D-03

ErrMax= 3.14D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.09D-02 BMatP= 8.60D-02

IDIUse=3 WtCom= 9.69D-01 WtEn= 3.14D-02

Coeff-Com: 0.836D-01-0.829D-01 0.141D+00 0.352D+00 0.506D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.195D-01 0.980D+00

Coeff: 0.809D-01-0.803D-01 0.137D+00 0.342D+00 0.521D+00

Gap= 0.034 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=7.78D-05 MaxDP=3.46D-03 DE=-1.75D-02 OVMax= 1.45D-02

Cycle 6 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 4.43D-05 CP: 9.86D-01 3.00D+00 5.31D-01 7.90D-01 5.98D-01

E= -1275.83937835139 Delta-E= -0.002221703775 Rises=F Damp=F

DIIS: error= 9.73D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.83937835139 IErMin= 6 ErrMin= 9.73D-04

ErrMax= 9.73D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.99D-04 BMatP= 1.09D-02

IDIUse=3 WtCom= 9.90D-01 WtEn= 9.73D-03

Coeff-Com: 0.505D-01-0.598D-01 0.445D-01 0.126D+00 0.290D+00 0.549D+00

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

Coeff: 0.500D-01-0.592D-01 0.441D-01 0.125D+00 0.287D+00 0.553D+00

Gap= 0.034 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=2.92D-05 MaxDP=1.23D-03 DE=-2.22D-03 OVMax= 8.45D-03

Cycle 7 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 2.42D-05 CP: 9.86D-01 3.00D+00 5.38D-01 7.82D-01 6.68D-01

CP: 7.98D-01

E= -1275.83962804045 Delta-E= -0.000249689056 Rises=F Damp=F

DIIS: error= 4.42D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.83962804045 IErMin= 7 ErrMin= 4.42D-04

ErrMax= 4.42D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.98D-05 BMatP= 9.99D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 4.42D-03

Coeff-Com: 0.894D-02-0.121D-01-0.743D-02-0.239D-01 0.373D-02 0.201D+00

Coeff-Com: 0.830D+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: 0.890D-02-0.120D-01-0.739D-02-0.238D-01 0.372D-02 0.200D+00

Coeff: 0.831D+00

Gap= 0.035 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.75D-05 MaxDP=9.25D-04 DE=-2.50D-04 OVMax= 9.69D-03

Cycle 8 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 1.25D-05 CP: 9.86D-01 3.00D+00 5.39D-01 7.83D-01 7.04D-01

CP: 1.02D+00 1.20D+00

E= -1275.83968887815 Delta-E= -0.000060837697 Rises=F Damp=F

DIIS: error= 2.42D-04 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.83968887815 IErMin= 8 ErrMin= 2.42D-04

ErrMax= 2.42D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.39D-05 BMatP= 8.98D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.42D-03

Coeff-Com: -0.974D-02 0.110D-01-0.133D-01-0.377D-01-0.731D-01-0.692D-01

Coeff-Com: 0.292D+00 0.900D+00

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

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

Coeff: -0.972D-02 0.110D-01-0.133D-01-0.376D-01-0.729D-01-0.690D-01

Coeff: 0.292D+00 0.900D+00

Gap= 0.035 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.72D-05 MaxDP=8.22D-04 DE=-6.08D-05 OVMax= 1.17D-02

Cycle 9 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 9.40D-06 CP: 9.86D-01 3.00D+00 5.39D-01 7.84D-01 7.28D-01

CP: 1.13D+00 1.64D+00 1.63D+00

E= -1275.83971665417 Delta-E= -0.000027776027 Rises=F Damp=F

DIIS: error= 2.31D-04 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.83971665417 IErMin= 9 ErrMin= 2.31D-04

ErrMax= 2.31D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.83D-05 BMatP= 2.39D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.31D-03

Coeff-Com: -0.111D-01 0.131D-01-0.732D-02-0.180D-01-0.548D-01-0.116D+00

Coeff-Com: -0.570D-01 0.667D+00 0.584D+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: -0.111D-01 0.131D-01-0.730D-02-0.180D-01-0.546D-01-0.116D+00

Coeff: -0.569D-01 0.665D+00 0.585D+00

Gap= 0.036 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.33D-05 MaxDP=5.30D-04 DE=-2.78D-05 OVMax= 1.00D-02

Cycle 10 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 5.56D-06 CP: 9.86D-01 3.00D+00 5.39D-01 7.85D-01 7.35D-01

CP: 1.21D+00 1.90D+00 2.35D+00 1.32D+00

E= -1275.83973331202 Delta-E= -0.000016657842 Rises=F Damp=F

DIIS: error= 1.51D-04 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.83973331202 IErMin=10 ErrMin= 1.51D-04

ErrMax= 1.51D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.25D-06 BMatP= 1.83D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.51D-03

Coeff-Com: -0.463D-02 0.543D-02-0.146D-02-0.120D-02-0.113D-01-0.335D-01

Coeff-Com: -0.713D-01 0.119D+00 0.247D+00 0.752D+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 0.000D+00 0.100D+01

Coeff: -0.463D-02 0.543D-02-0.146D-02-0.119D-02-0.112D-01-0.335D-01

Coeff: -0.712D-01 0.119D+00 0.247D+00 0.752D+00

Gap= 0.036 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.15D-05 MaxDP=4.27D-04 DE=-1.67D-05 OVMax= 9.22D-03

Cycle 11 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 2.07D-06 CP: 9.86D-01 3.00D+00 5.39D-01 7.85D-01 7.44D-01

CP: 1.26D+00 2.10D+00 2.93D+00 1.92D+00 1.66D+00

E= -1275.83974287914 Delta-E= -0.000009567123 Rises=F Damp=F

DIIS: error= 1.48D-04 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.83974287914 IErMin=11 ErrMin= 1.48D-04

ErrMax= 1.48D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.78D-06 BMatP= 3.25D-06

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.48D-03

Coeff-Com: 0.307D-03-0.438D-03 0.116D-02 0.470D-02 0.106D-01 0.237D-01

Coeff-Com: -0.240D-01-0.168D+00-0.483D-01 0.311D+00 0.889D+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 0.000D+00 0.000D+00 0.100D+01

Coeff: 0.306D-03-0.437D-03 0.116D-02 0.469D-02 0.105D-01 0.237D-01

Coeff: -0.240D-01-0.168D+00-0.483D-01 0.311D+00 0.889D+00

Gap= 0.036 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.48D-05 MaxDP=5.69D-04 DE=-9.57D-06 OVMax= 1.20D-02

Cycle 12 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 8.67D-06 CP: 9.86D-01 3.00D+00 5.39D-01 7.86D-01 7.54D-01

CP: 1.31D+00 2.35D+00 3.00D+00 2.65D+00 2.68D+00

CP: 2.07D+00

E= -1275.83975375845 Delta-E= -0.000010879315 Rises=F Damp=F

DIIS: error= 1.34D-04 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.83975375845 IErMin=12 ErrMin= 1.34D-04

ErrMax= 1.34D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.71D-06 BMatP= 1.78D-06

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.34D-03

Coeff-Com: 0.237D-02-0.277D-02 0.102D-02 0.156D-02 0.561D-02 0.241D-01

Coeff-Com: 0.158D-01-0.869D-01-0.810D-01-0.453D+00 0.495D+00 0.108D+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 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.100D+01

Coeff: 0.237D-02-0.277D-02 0.101D-02 0.156D-02 0.561D-02 0.241D-01

Coeff: 0.157D-01-0.867D-01-0.809D-01-0.452D+00 0.494D+00 0.108D+01

Gap= 0.036 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.94D-05 MaxDP=7.32D-04 DE=-1.09D-05 OVMax= 1.58D-02

Cycle 13 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 8.47D-06 CP: 9.86D-01 3.00D+00 5.38D-01 7.86D-01 7.67D-01

CP: 1.38D+00 2.66D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.42D+00

E= -1275.83976670632 Delta-E= -0.000012947869 Rises=F Damp=F

DIIS: error= 1.25D-04 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.83976670632 IErMin=13 ErrMin= 1.25D-04

ErrMax= 1.25D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.13D-06 BMatP= 1.71D-06

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.25D-03

Coeff-Com: 0.347D-02-0.393D-02-0.272D-03-0.543D-02-0.103D-01 0.400D-03

Coeff-Com: 0.543D-01 0.146D+00-0.113D-01-0.121D+01-0.448D+00 0.878D+00

Coeff-Com: 0.161D+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 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00

Coeff-En: 0.100D+01

Coeff: 0.347D-02-0.392D-02-0.271D-03-0.542D-02-0.103D-01 0.400D-03

Coeff: 0.542D-01 0.145D+00-0.113D-01-0.121D+01-0.448D+00 0.877D+00

Coeff: 0.161D+01

Gap= 0.036 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.77D-05 MaxDP=1.82D-03 DE=-1.29D-05 OVMax= 3.89D-02

Cycle 14 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 3.08D-05 CP: 9.86D-01 3.00D+00 5.38D-01 7.86D-01 7.96D-01

CP: 1.53D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

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

E= -1275.83979154132 Delta-E= -0.000024834999 Rises=F Damp=F

DIIS: error= 8.31D-05 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.83979154132 IErMin=14 ErrMin= 8.31D-05

ErrMax= 8.31D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.49D-07 BMatP= 1.13D-06

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

Coeff-Com: 0.168D-02-0.191D-02 0.440D-04-0.207D-02-0.590D-02-0.470D-02

Coeff-Com: 0.131D-01 0.947D-01 0.685D-02-0.148D+00-0.288D+00-0.664D+00

Coeff-Com: 0.980D+00 0.102D+01

Coeff: 0.168D-02-0.191D-02 0.440D-04-0.207D-02-0.590D-02-0.470D-02

Coeff: 0.131D-01 0.947D-01 0.685D-02-0.148D+00-0.288D+00-0.664D+00

Coeff: 0.980D+00 0.102D+01

Gap= 0.036 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.83D-05 MaxDP=1.09D-03 DE=-2.48D-05 OVMax= 2.31D-02

Cycle 15 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 8.23D-06 CP: 9.86D-01 3.00D+00 5.37D-01 7.86D-01 8.12D-01

CP: 1.62D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.87D+00

E= -1275.83980191836 Delta-E= -0.000010377039 Rises=F Damp=F

DIIS: error= 6.20D-05 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.83980191836 IErMin=15 ErrMin= 6.20D-05

ErrMax= 6.20D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.66D-07 BMatP= 8.49D-07

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

Coeff-Com: 0.988D-04-0.115D-03 0.392D-03 0.136D-02 0.948D-03 0.386D-03

Coeff-Com: -0.160D-01 0.384D-02-0.863D-02 0.524D+00 0.392D-01-0.102D+01

Coeff-Com: 0.311D-01 0.484D+00 0.955D+00

Coeff: 0.988D-04-0.115D-03 0.392D-03 0.136D-02 0.948D-03 0.386D-03

Coeff: -0.160D-01 0.384D-02-0.863D-02 0.524D+00 0.392D-01-0.102D+01

Coeff: 0.311D-01 0.484D+00 0.955D+00

Gap= 0.036 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.94D-05 MaxDP=7.50D-04 DE=-1.04D-05 OVMax= 1.58D-02

Cycle 16 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 1.26D-06 CP: 9.86D-01 3.00D+00 5.37D-01 7.85D-01 8.22D-01

CP: 1.67D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.46D+00 1.69D+00

E= -1275.83980717464 Delta-E= -0.000005256282 Rises=F Damp=F

DIIS: error= 4.55D-05 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1275.83980717464 IErMin=16 ErrMin= 4.55D-05

ErrMax= 4.55D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.60D-07 BMatP= 4.66D-07

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

Coeff-Com: -0.104D-02 0.120D-02-0.904D-04 0.975D-03 0.223D-02 0.374D-02

Coeff-Com: -0.131D-01-0.305D-01-0.443D-02 0.199D+00 0.198D+00-0.319D-01

Coeff-Com: -0.351D+00-0.810D+00 0.514D+00 0.132D+01

Coeff: -0.104D-02 0.120D-02-0.904D-04 0.975D-03 0.223D-02 0.374D-02

Coeff: -0.131D-01-0.305D-01-0.443D-02 0.199D+00 0.198D+00-0.319D-01

Coeff: -0.351D+00-0.810D+00 0.514D+00 0.132D+01

Gap= 0.036 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.17D-05 MaxDP=8.36D-04 DE=-5.26D-06 OVMax= 1.77D-02

Cycle 17 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 3.76D-06 CP: 9.86D-01 3.00D+00 5.36D-01 7.85D-01 8.34D-01

CP: 1.73D+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 2.50D+00

CP: 2.49D+00

E= -1275.83981117153 Delta-E= -0.000003996883 Rises=F Damp=F

DIIS: error= 2.55D-05 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=17 EnMin= -1275.83981117153 IErMin=17 ErrMin= 2.55D-05

ErrMax= 2.55D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.57D-07 BMatP= 2.60D-07

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

Coeff-Com: -0.109D-02 0.126D-02-0.260D-03 0.333D-03 0.192D-02 0.402D-02

Coeff-Com: -0.204D-03-0.345D-01 0.266D-02-0.183D+00 0.190D+00 0.468D+00

Coeff-Com: -0.212D+00-0.948D+00-0.194D+00 0.950D+00 0.956D+00

Coeff: -0.109D-02 0.126D-02-0.260D-03 0.333D-03 0.192D-02 0.402D-02

Coeff: -0.204D-03-0.345D-01 0.266D-02-0.183D+00 0.190D+00 0.468D+00

Coeff: -0.212D+00-0.948D+00-0.194D+00 0.950D+00 0.956D+00

Gap= 0.036 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.09D-05 MaxDP=8.09D-04 DE=-4.00D-06 OVMax= 1.71D-02

Cycle 18 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 1.26D-05 CP: 9.86D-01 3.00D+00 5.36D-01 7.85D-01 8.45D-01

CP: 1.79D+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: 3.00D+00 3.00D+00

E= -1275.83981304360 Delta-E= -0.000001872078 Rises=F Damp=F

DIIS: error= 9.43D-06 at cycle 18 NSaved= 18.

NSaved=18 IEnMin=18 EnMin= -1275.83981304360 IErMin=18 ErrMin= 9.43D-06

ErrMax= 9.43D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.38D-08 BMatP= 1.57D-07

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

Coeff-Com: -0.458D-03 0.534D-03-0.252D-03-0.513D-03-0.733D-03-0.260D-03

Coeff-Com: 0.808D-02 0.745D-02 0.882D-03-0.226D+00-0.507D-02 0.278D+00

Coeff-Com: 0.129D+00-0.190D+00-0.310D+00 0.312D-01 0.387D+00 0.891D+00

Coeff: -0.458D-03 0.534D-03-0.252D-03-0.513D-03-0.733D-03-0.260D-03

Coeff: 0.808D-02 0.745D-02 0.882D-03-0.226D+00-0.507D-02 0.278D+00

Coeff: 0.129D+00-0.190D+00-0.310D+00 0.312D-01 0.387D+00 0.891D+00

Gap= 0.036 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.92D-06 MaxDP=1.92D-04 DE=-1.87D-06 OVMax= 4.01D-03

Cycle 19 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 1.01D-06 CP: 9.86D-01 3.00D+00 5.36D-01 7.85D-01 8.47D-01

CP: 1.80D+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: 3.00D+00 3.00D+00 1.38D+00

E= -1275.83981320980 Delta-E= -0.000000166198 Rises=F Damp=F

DIIS: error= 3.52D-06 at cycle 19 NSaved= 19.

NSaved=19 IEnMin=19 EnMin= -1275.83981320980 IErMin=19 ErrMin= 3.52D-06

ErrMax= 3.52D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.51D-08 BMatP= 3.38D-08

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

Coeff-Com: -0.118D-03 0.141D-03-0.157D-03-0.547D-03-0.120D-02-0.144D-02

Coeff-Com: 0.668D-02 0.177D-01-0.167D-02-0.127D+00-0.686D-01 0.865D-01

Coeff-Com: 0.156D+00 0.835D-01-0.173D+00-0.176D+00 0.166D-01 0.569D+00

Coeff-Com: 0.613D+00

Coeff: -0.118D-03 0.141D-03-0.157D-03-0.547D-03-0.120D-02-0.144D-02

Coeff: 0.668D-02 0.177D-01-0.167D-02-0.127D+00-0.686D-01 0.865D-01

Coeff: 0.156D+00 0.835D-01-0.173D+00-0.176D+00 0.166D-01 0.569D+00

Coeff: 0.613D+00

Gap= 0.036 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.21D-06 MaxDP=1.63D-04 DE=-1.66D-07 OVMax= 3.43D-03

Cycle 20 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 3.01D-07 CP: 9.86D-01 3.00D+00 5.35D-01 7.85D-01 8.49D-01

CP: 1.81D+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: 3.00D+00 3.00D+00 1.71D+00 1.70D+00

E= -1275.83981325697 Delta-E= -0.000000047167 Rises=F Damp=F

DIIS: error= 3.18D-06 at cycle 20 NSaved= 20.

NSaved=20 IEnMin=20 EnMin= -1275.83981325697 IErMin=20 ErrMin= 3.18D-06

ErrMax= 3.18D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.40D-09 BMatP= 1.51D-08

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

Coeff-Com: 0.445D-04-0.502D-04-0.296D-04-0.183D-03-0.469D-03-0.338D-03

Coeff-Com: 0.262D-02 0.959D-02-0.607D-02-0.151D-01-0.451D-01 0.287D-01

Coeff-Com: 0.413D-01 0.628D-01-0.112D-01-0.802D-01-0.164D+00 0.131D+00

Coeff-Com: 0.419D+00 0.628D+00

Coeff: 0.445D-04-0.502D-04-0.296D-04-0.183D-03-0.469D-03-0.338D-03

Coeff: 0.262D-02 0.959D-02-0.607D-02-0.151D-01-0.451D-01 0.287D-01

Coeff: 0.413D-01 0.628D-01-0.112D-01-0.802D-01-0.164D+00 0.131D+00

Coeff: 0.419D+00 0.628D+00

Gap= 0.036 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.92D-07 MaxDP=1.02D-05 DE=-4.72D-08 OVMax= 1.92D-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= -1275.83981326000 Delta-E= -0.000000003033 Rises=F Damp=F

DIIS: error= 8.12D-07 at cycle 21 NSaved= 20.

NSaved=20 IEnMin=20 EnMin= -1275.83981326000 IErMin=20 ErrMin= 8.12D-07

ErrMax= 8.12D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.27D-10 BMatP= 7.40D-09

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

Coeff-Com: 0.193D-05-0.203D-04-0.924D-04-0.234D-03-0.437D-03 0.982D-04

Coeff-Com: 0.258D-02 0.113D-02 0.818D-03-0.956D-02-0.131D-01 0.119D-01

Coeff-Com: 0.171D-01 0.222D-02-0.129D-01-0.158D-01-0.714D-02 0.299D-01

Coeff-Com: 0.176D+00 0.818D+00

Coeff: 0.193D-05-0.203D-04-0.924D-04-0.234D-03-0.437D-03 0.982D-04

Coeff: 0.258D-02 0.113D-02 0.818D-03-0.956D-02-0.131D-01 0.119D-01

Coeff: 0.171D-01 0.222D-02-0.129D-01-0.158D-01-0.714D-02 0.299D-01

Coeff: 0.176D+00 0.818D+00

Gap= 0.036 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=6.36D-07 MaxDP=2.46D-05 DE=-3.03D-09 OVMax= 5.17D-04

Cycle 22 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 6.36D-07 CP: 1.00D+00

E= -1275.83981326100 Delta-E= -0.000000001001 Rises=F Damp=F

DIIS: error= 8.16D-07 at cycle 22 NSaved= 20.

NSaved=20 IEnMin=20 EnMin= -1275.83981326100 IErMin=19 ErrMin= 8.12D-07

ErrMax= 8.16D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.28D-10 BMatP= 6.27D-10

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

Coeff-Com: -0.717D-07 0.475D-05 0.242D-04-0.610D-04-0.620D-03-0.144D-02

Coeff-Com: 0.215D-02 0.452D-02 0.702D-02-0.126D-01-0.595D-02-0.114D-01

Coeff-Com: 0.652D-02 0.190D-01 0.363D-01-0.470D-01-0.115D+00-0.141D+00

Coeff-Com: 0.637D+00 0.622D+00

Coeff: -0.717D-07 0.475D-05 0.242D-04-0.610D-04-0.620D-03-0.144D-02

Coeff: 0.215D-02 0.452D-02 0.702D-02-0.126D-01-0.595D-02-0.114D-01

Coeff: 0.652D-02 0.190D-01 0.363D-01-0.470D-01-0.115D+00-0.141D+00

Coeff: 0.637D+00 0.622D+00

Gap= 0.036 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.90D-08 MaxDP=1.94D-06 DE=-1.00D-09 OVMax= 3.61D-05

Cycle 23 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 2.19D-08 CP: 1.00D+00 1.07D+00

E= -1275.83981326120 Delta-E= -0.000000000193 Rises=F Damp=F

DIIS: error= 5.16D-07 at cycle 23 NSaved= 20.

NSaved=20 IEnMin=20 EnMin= -1275.83981326120 IErMin=20 ErrMin= 5.16D-07

ErrMax= 5.16D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.70D-10 BMatP= 5.28D-10

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

Coeff-Com: 0.404D-05 0.240D-04 0.557D-04-0.928D-04-0.648D-03 0.498D-03

Coeff-Com: -0.185D-02 0.281D-02 0.247D-02-0.274D-02-0.958D-02-0.749D-03

Coeff-Com: 0.113D-01 0.203D-01-0.110D-01-0.548D-01-0.191D+00 0.142D+00

Coeff-Com: 0.226D+00 0.867D+00

Coeff: 0.404D-05 0.240D-04 0.557D-04-0.928D-04-0.648D-03 0.498D-03

Coeff: -0.185D-02 0.281D-02 0.247D-02-0.274D-02-0.958D-02-0.749D-03

Coeff: 0.113D-01 0.203D-01-0.110D-01-0.548D-01-0.191D+00 0.142D+00

Coeff: 0.226D+00 0.867D+00

Gap= 0.036 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.10D-08 MaxDP=1.08D-06 DE=-1.93D-10 OVMax= 9.30D-06

Cycle 24 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 1.17D-08 CP: 1.00D+00 1.09D+00 1.63D+00

E= -1275.83981326126 Delta-E= -0.000000000068 Rises=F Damp=F

DIIS: error= 1.56D-07 at cycle 24 NSaved= 20.

NSaved=20 IEnMin=20 EnMin= -1275.83981326126 IErMin=20 ErrMin= 1.56D-07

ErrMax= 1.56D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.15D-11 BMatP= 1.70D-10

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

Coeff-Com: 0.189D-05 0.425D-04 0.158D-03 0.130D-03-0.351D-03-0.301D-02

Coeff-Com: -0.896D-03 0.508D-02 0.148D-02-0.145D-02-0.329D-02 0.603D-03

Coeff-Com: 0.186D-02 0.964D-02 0.502D-02-0.707D-01-0.526D-01-0.522D-01

Coeff-Com: 0.323D+00 0.837D+00

Coeff: 0.189D-05 0.425D-04 0.158D-03 0.130D-03-0.351D-03-0.301D-02

Coeff: -0.896D-03 0.508D-02 0.148D-02-0.145D-02-0.329D-02 0.603D-03

Coeff: 0.186D-02 0.964D-02 0.502D-02-0.707D-01-0.526D-01-0.522D-01

Coeff: 0.323D+00 0.837D+00

Gap= 0.036 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=8.21D-08 MaxDP=3.20D-06 DE=-6.78D-11 OVMax= 6.68D-05

Cycle 25 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 8.49D-09 CP: 1.00D+00 9.58D-01 1.88D+00 1.10D+00

E= -1275.83981326129 Delta-E= -0.000000000021 Rises=F Damp=F

DIIS: error= 5.43D-08 at cycle 25 NSaved= 20.

NSaved=20 IEnMin=20 EnMin= -1275.83981326129 IErMin=20 ErrMin= 5.43D-08

ErrMax= 5.43D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.35D-12 BMatP= 2.15D-11

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

Coeff-Com: 0.145D-04 0.102D-03 0.127D-03-0.263D-03-0.114D-02-0.927D-03

Coeff-Com: 0.175D-02 0.121D-02 0.128D-02-0.158D-02-0.191D-02-0.231D-02

Coeff-Com: 0.596D-02 0.124D-01 0.198D-02-0.576D-01-0.646D-01-0.107D-01

Coeff-Com: 0.450D+00 0.666D+00

Coeff: 0.145D-04 0.102D-03 0.127D-03-0.263D-03-0.114D-02-0.927D-03

Coeff: 0.175D-02 0.121D-02 0.128D-02-0.158D-02-0.191D-02-0.231D-02

Coeff: 0.596D-02 0.124D-01 0.198D-02-0.576D-01-0.646D-01-0.107D-01

Coeff: 0.450D+00 0.666D+00

Gap= 0.036 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.55D-08 MaxDP=9.73D-07 DE=-2.14D-11 OVMax= 2.06D-05

Cycle 26 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 1.74D-09 CP: 1.00D+00 9.98D-01 1.94D+00 1.17D+00 9.92D-01

E= -1275.83981326128 Delta-E= 0.000000000010 Rises=F Damp=F

DIIS: error= 2.26D-08 at cycle 26 NSaved= 20.

NSaved=20 IEnMin=19 EnMin= -1275.83981326129 IErMin=20 ErrMin= 2.26D-08

ErrMax= 2.26D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.63D-13 BMatP= 3.35D-12

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

Coeff-Com: 0.167D-04 0.151D-04-0.450D-04 0.857D-04-0.174D-03 0.106D-03

Coeff-Com: 0.123D-03 0.740D-03-0.511D-04-0.920D-03-0.158D-02 0.863D-03

Coeff-Com: 0.577D-02 0.188D-01-0.209D-01-0.153D-01-0.676D-01-0.153D-01

Coeff-Com: 0.191D+00 0.904D+00

Coeff: 0.167D-04 0.151D-04-0.450D-04 0.857D-04-0.174D-03 0.106D-03

Coeff: 0.123D-03 0.740D-03-0.511D-04-0.920D-03-0.158D-02 0.863D-03

Coeff: 0.577D-02 0.188D-01-0.209D-01-0.153D-01-0.676D-01-0.153D-01

Coeff: 0.191D+00 0.904D+00

Gap= 0.036 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.96D-08 MaxDP=1.15D-06 DE= 1.00D-11 OVMax= 2.41D-05

Cycle 27 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 1.30D-09 CP: 1.00D+00 9.52D-01 1.96D+00 1.14D+00 1.35D+00

CP: 1.14D+00

E= -1275.83981326128 Delta-E= -0.000000000007 Rises=F Damp=F

DIIS: error= 3.31D-08 at cycle 27 NSaved= 20.

NSaved=20 IEnMin=18 EnMin= -1275.83981326129 IErMin=19 ErrMin= 2.26D-08

ErrMax= 3.31D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.06D-13 BMatP= 5.63D-13

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

Coeff-Com: -0.134D-04 0.292D-05 0.321D-03 0.549D-06-0.221D-03-0.244D-03

Coeff-Com: 0.425D-03 0.262D-03-0.477D-03-0.102D-02-0.437D-03 0.228D-02

Coeff-Com: 0.131D-01-0.964D-02 0.307D-02-0.225D-01-0.915D-01-0.639D-01

Coeff-Com: 0.542D+00 0.629D+00

Coeff: -0.134D-04 0.292D-05 0.321D-03 0.549D-06-0.221D-03-0.244D-03

Coeff: 0.425D-03 0.262D-03-0.477D-03-0.102D-02-0.437D-03 0.228D-02

Coeff: 0.131D-01-0.964D-02 0.307D-02-0.225D-01-0.915D-01-0.639D-01

Coeff: 0.542D+00 0.629D+00

Gap= 0.036 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=9.38D-09 MaxDP=3.61D-07 DE=-6.82D-12 OVMax= 7.60D-06

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

Error on total polarization charges = 0.06500

SCF Done: E(UB3LYP) = -1275.83981326 A.U. after 27 cycles

NFock= 27 Conv=0.94D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0410 S= 1.0136

<L.S>= 0.000000000000E+00

KE= 1.320695961116D+03 PE=-8.571608272908D+03 EE= 3.215198664255D+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 2.0410, after 2.0009

Leave Link 502 at Tue Sep 17 13:50:39 2019, MaxMem= 2415919104 cpu: 2645.5

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

(EU) (EU) (EU) (EU) (EU) (EU) (EU) (EU) (EU) (EU)

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

(?B) (?A) (?A) (?B) (?B) (?A) (?A) (?B) (BG) (?C)

(?C) (?C) (?D) (?D) (EG) (EG) (?B) (?B) (?D) (?D)

(?B) (?D) (?D) (?B) (?B) (AU) (EG) (EG) (?B) (EU)

(EU) (BU) (?B) (AU) (EG) (EG) (?E) (?E) (?F) (?A)

(?A) (?E) (?F) (?A) (?A) (?E) (?E) (?A) (?A) (?G)

(?G) (?E) (?A) (?A) (?F) (?E) (?E) (?G) (?G) (?F)

(?F) (?F) (?G)

Virtual (?G) (?F) (?F) (?F) (?G) (?G) (EU) (EU) (?F) (AG)

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

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Beta Orbitals:

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

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

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(BU) (?B) (?B) (BU) (BU) (?C) (BU) (?D) (?D) (?B)

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(BU) (?D) (?B) (?B) (?C) (BU) (BU) (?D) (?D) (?C)

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(?A) (?J) (?A) (EU) (EU) (EU) (EU) (?A) (?A) (?A)

(?A) (?A) (?A) (?A) (?A)

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

Alpha occ. eigenvalues -- -14.32219 -14.32219 -14.30380 -14.30380 -14.30353

Alpha occ. eigenvalues -- -14.30353 -14.30313 -14.30312 -10.25918 -10.25917

Alpha occ. eigenvalues -- -10.25785 -10.25785 -10.25119 -10.25119 -10.25061

Alpha occ. eigenvalues -- -10.25061 -10.19466 -10.19466 -10.19096 -10.19096

Alpha occ. eigenvalues -- -10.17566 -10.17566 -10.17402 -10.17402 -10.16594

Alpha occ. eigenvalues -- -10.16594 -10.16497 -10.16497 -1.00603 -0.99249

Alpha occ. eigenvalues -- -0.99139 -0.96516 -0.94108 -0.90056 -0.89878

Alpha occ. eigenvalues -- -0.86573 -0.80050 -0.79527 -0.79499 -0.79266

Alpha occ. eigenvalues -- -0.75513 -0.72114 -0.71971 -0.70453 -0.69262

Alpha occ. eigenvalues -- -0.68265 -0.68132 -0.63339 -0.61199 -0.58931

Alpha occ. eigenvalues -- -0.57773 -0.57380 -0.57041 -0.57033 -0.55515

Alpha occ. eigenvalues -- -0.55487 -0.54720 -0.54113 -0.53905 -0.53806

Alpha occ. eigenvalues -- -0.51857 -0.50688 -0.50664 -0.49148 -0.48749

Alpha occ. eigenvalues -- -0.46710 -0.45153 -0.45134 -0.44365 -0.43485

Alpha occ. eigenvalues -- -0.43430 -0.43229 -0.42861 -0.40908 -0.40713

Alpha occ. eigenvalues -- -0.40694 -0.40171 -0.39599 -0.39567 -0.39431

Alpha occ. eigenvalues -- -0.39404 -0.38065 -0.38060 -0.37678 -0.37654

Alpha occ. eigenvalues -- -0.37131 -0.36813 -0.32923 -0.32833 -0.32796

Alpha occ. eigenvalues -- -0.32487 -0.30696 -0.28129 -0.27608 -0.26584

Alpha occ. eigenvalues -- -0.26078 -0.25725 -0.25406 -0.25325 -0.25236

Alpha occ. eigenvalues -- -0.25091 -0.22643 -0.15045

Alpha virt. eigenvalues -- -0.11425 -0.05982 0.01766 0.03328 0.03740

Alpha virt. eigenvalues -- 0.03844 0.04495 0.04520 0.05170 0.05573

Alpha virt. eigenvalues -- 0.06957 0.06969 0.08163 0.08182 0.08916

Alpha virt. eigenvalues -- 0.09294 0.09773 0.09994 0.10004 0.10172

Alpha virt. eigenvalues -- 0.10446 0.10541 0.12890 0.13436 0.13568

Alpha virt. eigenvalues -- 0.13589 0.13636 0.13691 0.13713 0.14118

Alpha virt. eigenvalues -- 0.18193 0.20144 0.20604 0.20614 0.20680

Alpha virt. eigenvalues -- 0.21416 0.21723 0.21766 0.21910 0.22028

Alpha virt. eigenvalues -- 0.22656 0.22999 0.23047 0.25744 0.27041

Alpha virt. eigenvalues -- 0.27677 0.27726 0.28614 0.28861 0.29527

Alpha virt. eigenvalues -- 0.29595 0.30006 0.31357 0.31538 0.31563

Alpha virt. eigenvalues -- 0.31798 0.31910 0.32018 0.32080 0.32375

Alpha virt. eigenvalues -- 0.34616 0.35083 0.35166 0.35801 0.37447

Alpha virt. eigenvalues -- 0.37480 0.37662 0.38678 0.38705 0.38849

Alpha virt. eigenvalues -- 0.40030 0.40173 0.40198 0.40979 0.41547

Alpha virt. eigenvalues -- 0.43311 0.43394 0.43435 0.43668 0.43933

Alpha virt. eigenvalues -- 0.45268 0.46151 0.46255 0.46883 0.47935

Alpha virt. eigenvalues -- 0.48771 0.49068 0.49174 0.49441 0.49481

Alpha virt. eigenvalues -- 0.49550 0.51268 0.51340 0.51494 0.51613

Alpha virt. eigenvalues -- 0.52868 0.53665 0.53691 0.53716 0.54204

Alpha virt. eigenvalues -- 0.56325 0.56399 0.56443 0.56591 0.57228

Alpha virt. eigenvalues -- 0.57260 0.57542 0.58305 0.58337 0.58720

Alpha virt. eigenvalues -- 0.58819 0.59435 0.59841 0.59881 0.60459

Alpha virt. eigenvalues -- 0.61632 0.62719 0.63152 0.63172 0.63286

Alpha virt. eigenvalues -- 0.63297 0.63468 0.64980 0.65106 0.65128

Alpha virt. eigenvalues -- 0.68016 0.68082 0.68622 0.68797 0.68848

Alpha virt. eigenvalues -- 0.69444 0.69533 0.69974 0.70850 0.71639

Alpha virt. eigenvalues -- 0.73275 0.73478 0.73533 0.74730 0.75332

Alpha virt. eigenvalues -- 0.75954 0.76008 0.77847 0.77879 0.79142

Alpha virt. eigenvalues -- 0.79818 0.79924 0.80905 0.80973 0.81249

Alpha virt. eigenvalues -- 0.81529 0.81569 0.82254 0.82704 0.85221

Alpha virt. eigenvalues -- 0.85319 0.85363 0.87006 0.88779 0.88840

Alpha virt. eigenvalues -- 0.88850 0.89751 0.94463 0.96860 0.96893

Alpha virt. eigenvalues -- 0.97647 0.97901 0.99862 0.99919 1.00578

Alpha virt. eigenvalues -- 1.03272 1.03328 1.03962 1.04964 1.04999

Alpha virt. eigenvalues -- 1.06611 1.07948 1.08508 1.08539 1.10378

Alpha virt. eigenvalues -- 1.10564 1.13428 1.13597 1.13650 1.13741

Alpha virt. eigenvalues -- 1.13744 1.13775 1.13882 1.14343 1.15016

Alpha virt. eigenvalues -- 1.18123 1.18629 1.19229 1.19263 1.20745

Alpha virt. eigenvalues -- 1.21058 1.21168 1.23557 1.24083 1.27652

Alpha virt. eigenvalues -- 1.28482 1.29228 1.29308 1.30708 1.36389

Alpha virt. eigenvalues -- 1.36473 1.37261 1.38493 1.39131 1.40483

Alpha virt. eigenvalues -- 1.41013 1.41047 1.42126 1.42357 1.43928

Alpha virt. eigenvalues -- 1.45242 1.49491 1.49837 1.49929 1.51080

Alpha virt. eigenvalues -- 1.51104 1.51160 1.51296 1.52035 1.52051

Alpha virt. eigenvalues -- 1.52078 1.53003 1.53756 1.54779 1.54828

Alpha virt. eigenvalues -- 1.55353 1.55957 1.56043 1.57055 1.58299

Alpha virt. eigenvalues -- 1.60152 1.60717 1.60768 1.62203 1.62992

Alpha virt. eigenvalues -- 1.63006 1.63191 1.67066 1.68307 1.68338

Alpha virt. eigenvalues -- 1.68414 1.69177 1.69233 1.69573 1.70839

Alpha virt. eigenvalues -- 1.71863 1.71882 1.73898 1.75764 1.75791

Alpha virt. eigenvalues -- 1.75923 1.79646 1.79846 1.79893 1.80145

Alpha virt. eigenvalues -- 1.84872 1.86406 1.86490 1.87093 1.88564

Alpha virt. eigenvalues -- 1.90191 1.90229 1.90479 1.91507 1.93998

Alpha virt. eigenvalues -- 1.95204 1.96309 1.96463 1.96872 2.00563

Alpha virt. eigenvalues -- 2.00696 2.00725 2.00811 2.01754 2.01876

Alpha virt. eigenvalues -- 2.02055 2.02135 2.05393 2.06495 2.08258

Alpha virt. eigenvalues -- 2.09050 2.09087 2.12861 2.12879 2.15012

Alpha virt. eigenvalues -- 2.15534 2.15538 2.17247 2.17306 2.20353

Alpha virt. eigenvalues -- 2.27336 2.28863 2.29119 2.29183 2.29404

Alpha virt. eigenvalues -- 2.29732 2.32947 2.33054 2.34944 2.35164

Alpha virt. eigenvalues -- 2.35212 2.36124 2.37490 2.37542 2.37607

Alpha virt. eigenvalues -- 2.39077 2.39100 2.39134 2.39587 2.43698

Alpha virt. eigenvalues -- 2.47381 2.47418 2.47432 2.47918 2.47924

Alpha virt. eigenvalues -- 2.47972 2.48716 2.49075 2.55007 2.55578

Alpha virt. eigenvalues -- 2.55635 2.55793 2.57695 2.57717 2.59027

Alpha virt. eigenvalues -- 2.60062 2.60111 2.62961 2.63522 2.64654

Alpha virt. eigenvalues -- 2.66109 2.67195 2.70363 2.70427 2.71666

Alpha virt. eigenvalues -- 2.72505 2.72561 2.72601 2.75373 2.75444

Alpha virt. eigenvalues -- 2.76308 2.79211 2.82788 2.83545 2.83756

Alpha virt. eigenvalues -- 2.84053 2.84113 2.84798 2.84882 2.85151

Alpha virt. eigenvalues -- 2.91440 2.91519 2.92739 2.93437 2.95483

Alpha virt. eigenvalues -- 2.96700 2.96739 3.01100 3.03350 3.04289

Alpha virt. eigenvalues -- 3.04381 3.05524 3.12243 3.12438 3.12524

Alpha virt. eigenvalues -- 3.13025 3.13104 3.13389 3.13984 3.14140

Alpha virt. eigenvalues -- 3.15744 3.16379 3.16483 3.17846 3.20406

Alpha virt. eigenvalues -- 3.20519 3.20913 3.22109 3.24223 3.26363

Alpha virt. eigenvalues -- 3.28074 3.28162 3.28259 3.30306 3.30344

Alpha virt. eigenvalues -- 3.36165 3.37471 3.38612 3.38646 3.39085

Alpha virt. eigenvalues -- 3.53159 3.57404 3.57436 3.69913 3.72287

Alpha virt. eigenvalues -- 3.72340 3.72348 3.76215 3.77650 3.78180

Alpha virt. eigenvalues -- 3.78184 3.78715 3.81214 3.81900 3.82024

Alpha virt. eigenvalues -- 3.87199 3.88004 3.88028 3.88190 3.91221

Alpha virt. eigenvalues -- 4.04588 4.04815 4.05210 4.05400 4.11386

Alpha virt. eigenvalues -- 4.12298 4.12461 4.18619 4.28219 4.35070

Alpha virt. eigenvalues -- 4.35554 4.37690 4.46117 4.51526 4.61473

Alpha virt. eigenvalues -- 4.61500 4.99542 5.02680 5.02940 5.11342

Alpha virt. eigenvalues -- 5.15076 5.32820 5.33317 5.50283 7.78590

Alpha virt. eigenvalues -- 7.78611 7.89784 7.95371 8.22999 11.19706

Alpha virt. eigenvalues -- 23.43296 23.45698 23.45797 23.47113 23.66375

Alpha virt. eigenvalues -- 23.66938 23.67036 23.67123 23.81061 23.81809

Alpha virt. eigenvalues -- 23.82158 23.83085 23.85696 23.86623 23.87001

Alpha virt. eigenvalues -- 23.87009 24.09375 24.09808 24.09912 24.10562

Alpha virt. eigenvalues -- 35.56575 35.60881 35.61255 35.62148 35.67619

Alpha virt. eigenvalues -- 35.68329 35.69492 35.69711

Beta occ. eigenvalues -- -14.32482 -14.32482 -14.30416 -14.30416 -14.30339

Beta occ. eigenvalues -- -14.30338 -14.30047 -14.30047 -10.25702 -10.25702

Beta occ. eigenvalues -- -10.25567 -10.25567 -10.24661 -10.24660 -10.24604

Beta occ. eigenvalues -- -10.24604 -10.19450 -10.19450 -10.18883 -10.18883

Beta occ. eigenvalues -- -10.17638 -10.17638 -10.17295 -10.17295 -10.16593

Beta occ. eigenvalues -- -10.16593 -10.16509 -10.16509 -1.00165 -0.98878

Beta occ. eigenvalues -- -0.98625 -0.96105 -0.93685 -0.90023 -0.89234

Beta occ. eigenvalues -- -0.86398 -0.79822 -0.79375 -0.79252 -0.79072

Beta occ. eigenvalues -- -0.74737 -0.71709 -0.71587 -0.70335 -0.69027

Beta occ. eigenvalues -- -0.67809 -0.67766 -0.62885 -0.60694 -0.58818

Beta occ. eigenvalues -- -0.57656 -0.57293 -0.56801 -0.56712 -0.55492

Beta occ. eigenvalues -- -0.55472 -0.54538 -0.54030 -0.53589 -0.53485

Beta occ. eigenvalues -- -0.51650 -0.50540 -0.50456 -0.48913 -0.48608

Beta occ. eigenvalues -- -0.45431 -0.44286 -0.44042 -0.43815 -0.43410

Beta occ. eigenvalues -- -0.43349 -0.42775 -0.42465 -0.40624 -0.40343

Beta occ. eigenvalues -- -0.40167 -0.39983 -0.39551 -0.39289 -0.39225

Beta occ. eigenvalues -- -0.38343 -0.37887 -0.37582 -0.37518 -0.37035

Beta occ. eigenvalues -- -0.36720 -0.36666 -0.32858 -0.32724 -0.31518

Beta occ. eigenvalues -- -0.30601 -0.30387 -0.28281 -0.27232 -0.26023

Beta occ. eigenvalues -- -0.25943 -0.25664 -0.24968 -0.24891 -0.24872

Beta occ. eigenvalues -- -0.24680

Beta virt. eigenvalues -- -0.16441 -0.10238 -0.09087 -0.03990 0.03602

Beta virt. eigenvalues -- 0.03745 0.04569 0.04605 0.05179 0.05303

Beta virt. eigenvalues -- 0.05610 0.06442 0.06970 0.06995 0.08216

Beta virt. eigenvalues -- 0.08222 0.09329 0.10023 0.10037 0.10236

Beta virt. eigenvalues -- 0.10297 0.10785 0.11695 0.12005 0.12901

Beta virt. eigenvalues -- 0.13595 0.13611 0.13657 0.13657 0.14139

Beta virt. eigenvalues -- 0.14158 0.14468 0.18527 0.20344 0.20750

Beta virt. eigenvalues -- 0.20857 0.21038 0.21921 0.22037 0.22119

Beta virt. eigenvalues -- 0.22176 0.22384 0.22965 0.23424 0.23548

Beta virt. eigenvalues -- 0.26087 0.27414 0.27802 0.27942 0.28836

Beta virt. eigenvalues -- 0.29418 0.29891 0.30000 0.30408 0.31478

Beta virt. eigenvalues -- 0.31644 0.31724 0.32103 0.32163 0.32200

Beta virt. eigenvalues -- 0.32267 0.32565 0.34734 0.35398 0.35470

Beta virt. eigenvalues -- 0.36060 0.37702 0.37719 0.37968 0.39187

Beta virt. eigenvalues -- 0.39607 0.39826 0.40259 0.40384 0.40449

Beta virt. eigenvalues -- 0.41248 0.42240 0.43602 0.43619 0.43992

Beta virt. eigenvalues -- 0.44393 0.44664 0.45529 0.46627 0.46662

Beta virt. eigenvalues -- 0.47149 0.48161 0.49302 0.49371 0.49423

Beta virt. eigenvalues -- 0.49695 0.49755 0.49769 0.51504 0.51859

Beta virt. eigenvalues -- 0.52085 0.52243 0.53543 0.53785 0.53860

Beta virt. eigenvalues -- 0.53875 0.54303 0.56446 0.56564 0.56614

Beta virt. eigenvalues -- 0.56741 0.57365 0.57378 0.58001 0.58449

Beta virt. eigenvalues -- 0.58513 0.58813 0.58988 0.59501 0.59995

Beta virt. eigenvalues -- 0.60074 0.60621 0.61812 0.62918 0.63403

Beta virt. eigenvalues -- 0.63486 0.63587 0.63835 0.63918 0.65160

Beta virt. eigenvalues -- 0.65225 0.65255 0.68298 0.68698 0.68749

Beta virt. eigenvalues -- 0.68953 0.69104 0.69417 0.69834 0.70222

Beta virt. eigenvalues -- 0.71089 0.71959 0.73553 0.73750 0.73821

Beta virt. eigenvalues -- 0.74898 0.75631 0.76132 0.76182 0.78056

Beta virt. eigenvalues -- 0.78124 0.79212 0.80006 0.80254 0.80866

Beta virt. eigenvalues -- 0.81526 0.81646 0.81690 0.81808 0.82389

Beta virt. eigenvalues -- 0.82864 0.85367 0.85479 0.85552 0.87141

Beta virt. eigenvalues -- 0.88975 0.88983 0.89119 0.89943 0.94728

Beta virt. eigenvalues -- 0.96976 0.96995 0.97922 0.98059 1.00035

Beta virt. eigenvalues -- 1.00143 1.01214 1.03760 1.03872 1.04087

Beta virt. eigenvalues -- 1.05223 1.05269 1.06941 1.08114 1.09179

Beta virt. eigenvalues -- 1.09282 1.10655 1.10974 1.13566 1.13784

Beta virt. eigenvalues -- 1.13899 1.14114 1.14523 1.14592 1.14658

Beta virt. eigenvalues -- 1.15055 1.15891 1.18445 1.19320 1.19364

Beta virt. eigenvalues -- 1.19625 1.21041 1.21820 1.21915 1.23655

Beta virt. eigenvalues -- 1.24189 1.27812 1.29191 1.29470 1.29552

Beta virt. eigenvalues -- 1.30872 1.37194 1.37268 1.37607 1.39335

Beta virt. eigenvalues -- 1.39443 1.41157 1.41214 1.41247 1.42320

Beta virt. eigenvalues -- 1.42833 1.44259 1.45548 1.49577 1.49911

Beta virt. eigenvalues -- 1.50068 1.51165 1.51199 1.51256 1.51369

Beta virt. eigenvalues -- 1.52104 1.52114 1.52133 1.53155 1.54320

Beta virt. eigenvalues -- 1.54981 1.55014 1.55540 1.56280 1.56311

Beta virt. eigenvalues -- 1.57453 1.58705 1.60340 1.61150 1.61187

Beta virt. eigenvalues -- 1.62335 1.63203 1.63267 1.63523 1.67213

Beta virt. eigenvalues -- 1.68492 1.68607 1.69070 1.69342 1.69501

Beta virt. eigenvalues -- 1.69831 1.71018 1.72532 1.72760 1.74137

Beta virt. eigenvalues -- 1.75994 1.76117 1.76843 1.80080 1.80159

Beta virt. eigenvalues -- 1.80280 1.80423 1.85075 1.86645 1.86762

Beta virt. eigenvalues -- 1.87648 1.88826 1.90703 1.90788 1.90907

Beta virt. eigenvalues -- 1.92139 1.94477 1.95677 1.96851 1.96958

Beta virt. eigenvalues -- 1.97191 2.00924 2.01000 2.01218 2.01243

Beta virt. eigenvalues -- 2.02110 2.02463 2.02703 2.02954 2.05592

Beta virt. eigenvalues -- 2.07028 2.08643 2.09058 2.09427 2.13277

Beta virt. eigenvalues -- 2.13329 2.15381 2.15968 2.16173 2.17473

Beta virt. eigenvalues -- 2.17896 2.20888 2.27472 2.29190 2.29280

Beta virt. eigenvalues -- 2.29458 2.29806 2.29854 2.33109 2.33793

Beta virt. eigenvalues -- 2.35018 2.35230 2.35331 2.36192 2.37729

Beta virt. eigenvalues -- 2.38033 2.38271 2.39183 2.39284 2.39479

Beta virt. eigenvalues -- 2.40181 2.43856 2.47646 2.47681 2.47827

Beta virt. eigenvalues -- 2.47972 2.48056 2.48298 2.49222 2.49358

Beta virt. eigenvalues -- 2.55050 2.55567 2.55898 2.55976 2.57757

Beta virt. eigenvalues -- 2.57930 2.59735 2.60770 2.60793 2.63572

Beta virt. eigenvalues -- 2.63642 2.64793 2.66795 2.67284 2.70914

Beta virt. eigenvalues -- 2.71084 2.72242 2.72548 2.72756 2.72824

Beta virt. eigenvalues -- 2.76240 2.76866 2.77376 2.80509 2.83725

Beta virt. eigenvalues -- 2.84256 2.84610 2.84800 2.84920 2.85034

Beta virt. eigenvalues -- 2.85261 2.85274 2.91581 2.91680 2.92911

Beta virt. eigenvalues -- 2.94207 2.95599 2.97597 2.97730 3.02190

Beta virt. eigenvalues -- 3.03520 3.04410 3.04525 3.05654 3.12337

Beta virt. eigenvalues -- 3.12613 3.12633 3.13139 3.13269 3.13537

Beta virt. eigenvalues -- 3.14091 3.14343 3.15946 3.16482 3.16583

Beta virt. eigenvalues -- 3.17904 3.20517 3.20710 3.21034 3.22222

Beta virt. eigenvalues -- 3.24342 3.26463 3.28190 3.28286 3.28413

Beta virt. eigenvalues -- 3.30447 3.30500 3.36320 3.37548 3.38653

Beta virt. eigenvalues -- 3.38793 3.39198 3.53416 3.57633 3.57660

Beta virt. eigenvalues -- 3.70126 3.72523 3.72580 3.72584 3.76405

Beta virt. eigenvalues -- 3.77907 3.78408 3.78433 3.78953 3.81239

Beta virt. eigenvalues -- 3.81496 3.82581 3.87267 3.87579 3.88418

Beta virt. eigenvalues -- 3.89153 3.91400 4.04695 4.05144 4.05323

Beta virt. eigenvalues -- 4.05722 4.11490 4.12409 4.12671 4.18855

Beta virt. eigenvalues -- 4.28401 4.35349 4.35947 4.38105 4.46308

Beta virt. eigenvalues -- 4.51627 4.61581 4.61629 4.99878 5.02964

Beta virt. eigenvalues -- 5.03343 5.11681 5.15438 5.33132 5.33734

Beta virt. eigenvalues -- 5.50649 7.78601 7.78621 7.89783 7.95373

Beta virt. eigenvalues -- 8.23003 11.19713 23.43386 23.45775 23.45877

Beta virt. eigenvalues -- 23.47185 23.66419 23.66982 23.67073 23.67161

Beta virt. eigenvalues -- 23.81375 23.82080 23.82565 23.83414 23.86117

Beta virt. eigenvalues -- 23.86957 23.87420 23.87472 24.09455 24.09881

Beta virt. eigenvalues -- 24.10000 24.10642 35.56546 35.60788 35.61287

Beta virt. eigenvalues -- 35.62118 35.67486 35.68120 35.69677 35.69975

Condensed to atoms (all electrons):

1 2 3 4 5 6

1 C 4.645793 0.383538 -0.130842 -0.057487 0.419931 -0.001003

2 N 0.383538 7.135187 0.399856 -0.059276 -0.100987 -0.086525

3 C -0.130842 0.399856 4.612379 0.395683 -0.065610 0.556637

4 C -0.057487 -0.059276 0.395683 5.081322 0.616740 -0.079868

5 C 0.419931 -0.100987 -0.065610 0.616740 5.122412 0.005013

6 N -0.001003 -0.086525 0.556637 -0.079868 0.005013 6.654552

7 C -0.001147 -0.003506 -0.089439 0.004321 -0.000407 0.510746

8 N 0.000449 -0.018988 -0.004193 -0.000096 -0.000197 -0.079270

9 C 0.000005 0.000313 -0.000989 0.000014 -0.000003 0.001227

10 C -0.000003 -0.000084 0.000015 0.000015 0.000000 0.003850

11 C 0.000016 0.000263 0.004348 -0.000291 0.000010 -0.047181

12 N 0.513464 -0.073527 0.000162 0.003539 -0.041791 -0.000156

13 C 0.003817 -0.000089 0.000019 0.000017 -0.000335 -0.000000

14 C -0.000275 -0.000197 -0.000003 0.000000 0.000011 -0.000000

15 C -0.000969 0.000498 -0.000008 -0.000003 0.000020 -0.000001

16 N -0.001805 -0.021222 0.000371 -0.000093 0.000249 -0.000001

17 C -0.101857 -0.002628 -0.000803 0.000139 0.003686 -0.000032

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

19 N 0.000168 -0.003284 0.000203 0.000002 0.000003 -0.000001

20 C -0.000047 0.000203 -0.000012 -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 -0.000006 0.000168 -0.000047 -0.000000 -0.000000 -0.000026

24 N -0.000001 -0.000005 -0.000024 -0.000000 -0.000000 -0.000156

25 Zn -0.016064 0.117187 -0.017088 -0.000775 -0.000617 -0.005602

26 C 0.009718 0.009064 -0.067920 0.263816 -0.056886 0.015348

27 H -0.048122 0.006145 0.009693 -0.042969 0.395047 -0.000010

28 C 0.000000 0.000001 0.000002 -0.000000 0.000000 -0.000021

29 H 0.000001 0.000078 -0.000073 -0.000161 -0.000005 0.006670

30 C -0.000363 0.000058 0.000000 -0.000000 -0.000039 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 0.000247 -0.000230 0.006116 -0.041902 -0.005504 0.000087

35 H -0.000073 0.000386 -0.005092 -0.045981 -0.000244 0.004671

36 H -0.000073 0.000386 -0.005092 -0.045981 -0.000244 0.004671

37 H -0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000007

38 H -0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000007

39 H -0.000000 -0.000000 0.000001 0.000000 0.000000 -0.000011

40 H -0.000003 0.000012 -0.000000 0.000000 -0.000017 0.000000

41 H -0.000003 0.000012 -0.000000 0.000000 -0.000017 0.000000

42 H 0.000037 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 -0.001147 0.000449 0.000005 -0.000003 0.000016 0.513464

2 N -0.003506 -0.018988 0.000313 -0.000084 0.000263 -0.073527

3 C -0.089439 -0.004193 -0.000989 0.000015 0.004348 0.000162

4 C 0.004321 -0.000096 0.000014 0.000015 -0.000291 0.003539

5 C -0.000407 -0.000197 -0.000003 0.000000 0.000010 -0.041791

6 N 0.510746 -0.079270 0.001227 0.003850 -0.047181 -0.000156

7 C 4.579691 0.418146 -0.129629 -0.050475 0.412275 -0.000018

8 N 0.418146 7.138018 0.363131 -0.066450 -0.092875 -0.000005

9 C -0.129629 0.363131 4.678504 0.404045 -0.073537 -0.000001

10 C -0.050475 -0.066450 0.404045 5.044501 0.618523 -0.000000

11 C 0.412275 -0.092875 -0.073537 0.618523 5.144075 -0.000000

12 N -0.000018 -0.000005 -0.000001 -0.000000 -0.000000 6.578473

13 C -0.000000 0.000002 -0.000000 0.000000 -0.000000 -0.072203

14 C -0.000000 0.000003 -0.000000 -0.000000 0.000000 0.004553

15 C -0.000005 0.000151 -0.000047 -0.000000 -0.000000 -0.001932

16 N 0.000151 -0.003290 0.000221 0.000002 0.000003 -0.080607

17 C -0.000047 0.000221 -0.000013 -0.000000 -0.000000 0.558308

18 N -0.000001 -0.000001 -0.000032 -0.000000 -0.000000 -0.000156

19 N 0.000498 -0.021222 -0.002628 -0.000089 -0.000197 -0.000005

20 C -0.000008 0.000371 -0.000803 0.000019 -0.000003 -0.000024

21 C -0.000003 -0.000093 0.000139 0.000017 0.000000 -0.000000

22 C 0.000020 0.000249 0.003686 -0.000335 0.000011 -0.000000

23 C -0.000969 -0.001805 -0.101857 0.003817 -0.000275 -0.000001

24 N -0.001932 -0.080607 0.558308 -0.072203 0.004553 0.000000

25 Zn -0.016393 0.117686 -0.017072 -0.000679 -0.000485 -0.005180

26 C -0.000309 0.000062 0.000000 0.000000 -0.000043 -0.000017

27 H 0.000010 0.000001 0.000000 0.000000 -0.000000 0.006204

28 C 0.009463 0.008839 -0.069055 0.265326 -0.055165 -0.000000

29 H -0.048824 0.006390 0.009749 -0.042812 0.394852 0.000000

30 C 0.000000 -0.000000 0.000000 -0.000000 -0.000000 0.014189

31 H 0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000007

32 C 0.000000 0.000001 0.000002 -0.000000 0.000000 0.000000

33 H 0.000001 0.000073 -0.000138 -0.000145 -0.000004 -0.000000

34 H 0.000039 0.000000 0.000000 0.000000 -0.000001 -0.000011

35 H -0.000029 0.000012 0.000000 0.000000 -0.000031 0.000008

36 H -0.000029 0.000012 0.000000 0.000000 -0.000031 0.000008

37 H -0.000163 0.000419 -0.005136 -0.043694 -0.000287 -0.000000

38 H -0.000163 0.000419 -0.005136 -0.043694 -0.000287 -0.000000

39 H 0.000242 -0.000239 0.006091 -0.041603 -0.005411 -0.000000

40 H 0.000000 0.000000 0.000000 0.000000 -0.000000 0.003788

41 H 0.000000 0.000000 0.000000 0.000000 -0.000000 0.003788

42 H 0.000000 -0.000000 0.000000 0.000000 0.000000 0.000063

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 0.003817 -0.000275 -0.000969 -0.001805 -0.101857 -0.000026

2 N -0.000089 -0.000197 0.000498 -0.021222 -0.002628 -0.000001

3 C 0.000019 -0.000003 -0.000008 0.000371 -0.000803 -0.000001

4 C 0.000017 0.000000 -0.000003 -0.000093 0.000139 -0.000000

5 C -0.000335 0.000011 0.000020 0.000249 0.003686 -0.000000

6 N -0.000000 -0.000000 -0.000001 -0.000001 -0.000032 0.000000

7 C -0.000000 -0.000000 -0.000005 0.000151 -0.000047 -0.000001

8 N 0.000002 0.000003 0.000151 -0.003290 0.000221 -0.000001

9 C -0.000000 -0.000000 -0.000047 0.000221 -0.000013 -0.000032

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 -0.072203 0.004553 -0.001932 -0.080607 0.558308 -0.000156

13 C 5.044501 0.618523 -0.050475 -0.066450 0.404045 0.003850

14 C 0.618523 5.144075 0.412275 -0.092875 -0.073537 -0.047181

15 C -0.050475 0.412275 4.579691 0.418146 -0.129629 0.510746

16 N -0.066450 -0.092875 0.418146 7.138018 0.363131 -0.079270

17 C 0.404045 -0.073537 -0.129629 0.363131 4.678504 0.001227

18 N 0.003850 -0.047181 0.510746 -0.079270 0.001227 6.654552

19 N -0.000084 0.000263 -0.003506 -0.018988 0.000313 -0.086525

20 C 0.000015 0.004348 -0.089439 -0.004193 -0.000989 0.556637

21 C 0.000015 -0.000291 0.004321 -0.000096 0.000014 -0.079868

22 C 0.000000 0.000010 -0.000407 -0.000197 -0.000003 0.005013

23 C -0.000003 0.000016 -0.001147 0.000449 0.000005 -0.001003

24 N -0.000000 -0.000000 -0.000018 -0.000005 -0.000001 -0.000156

25 Zn -0.000679 -0.000485 -0.016393 0.117686 -0.017072 -0.005602

26 C -0.000000 0.000000 0.000000 0.000001 0.000002 -0.000000

27 H -0.000145 -0.000004 0.000001 0.000073 -0.000138 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 0.265326 -0.055165 0.009463 0.008839 -0.069055 -0.000021

31 H -0.042812 0.394852 -0.048824 0.006390 0.009749 0.006670

32 C 0.000000 -0.000043 -0.000309 0.000062 0.000000 0.015348

33 H 0.000000 -0.000000 0.000010 0.000001 0.000000 -0.000010

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 -0.043694 -0.000287 -0.000163 0.000419 -0.005136 0.000007

41 H -0.043694 -0.000287 -0.000163 0.000419 -0.005136 0.000007

42 H -0.041603 -0.005411 0.000242 -0.000239 0.006091 -0.000011

43 H 0.000000 -0.000031 -0.000029 0.000012 0.000000 0.004671

44 H 0.000000 -0.000031 -0.000029 0.000012 0.000000 0.004671

45 H 0.000000 -0.000001 0.000039 0.000000 0.000000 0.000087

19 20 21 22 23 24

1 C 0.000168 -0.000047 -0.000000 -0.000000 -0.000006 -0.000001

2 N -0.003284 0.000203 0.000002 0.000003 0.000168 -0.000005

3 C 0.000203 -0.000012 -0.000000 -0.000000 -0.000047 -0.000024

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 -0.000001 -0.000001 -0.000000 -0.000000 -0.000026 -0.000156

7 C 0.000498 -0.000008 -0.000003 0.000020 -0.000969 -0.001932

8 N -0.021222 0.000371 -0.000093 0.000249 -0.001805 -0.080607

9 C -0.002628 -0.000803 0.000139 0.003686 -0.101857 0.558308

10 C -0.000089 0.000019 0.000017 -0.000335 0.003817 -0.072203

11 C -0.000197 -0.000003 0.000000 0.000011 -0.000275 0.004553

12 N -0.000005 -0.000024 -0.000000 -0.000000 -0.000001 0.000000

13 C -0.000084 0.000015 0.000015 0.000000 -0.000003 -0.000000

14 C 0.000263 0.004348 -0.000291 0.000010 0.000016 -0.000000

15 C -0.003506 -0.089439 0.004321 -0.000407 -0.001147 -0.000018

16 N -0.018988 -0.004193 -0.000096 -0.000197 0.000449 -0.000005

17 C 0.000313 -0.000989 0.000014 -0.000003 0.000005 -0.000001

18 N -0.086525 0.556637 -0.079868 0.005013 -0.001003 -0.000156

19 N 7.135187 0.399856 -0.059276 -0.100987 0.383538 -0.073527

20 C 0.399856 4.612379 0.395683 -0.065610 -0.130842 0.000162

21 C -0.059276 0.395683 5.081322 0.616740 -0.057487 0.003539

22 C -0.100987 -0.065610 0.616740 5.122412 0.419931 -0.041791

23 C 0.383538 -0.130842 -0.057487 0.419931 4.645793 0.513464

24 N -0.073527 0.000162 0.003539 -0.041791 0.513464 6.578473

25 Zn 0.117187 -0.017088 -0.000775 -0.000617 -0.016064 -0.005180

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 0.000058 0.000000 -0.000000 -0.000039 -0.000363 0.014189

29 H 0.000001 0.000000 0.000000 -0.000000 0.000011 -0.000007

30 C 0.000001 0.000002 -0.000000 0.000000 0.000000 -0.000000

31 H 0.000078 -0.000073 -0.000161 -0.000005 0.000001 0.000000

32 C 0.009064 -0.067920 0.263816 -0.056886 0.009718 -0.000017

33 H 0.006145 0.009693 -0.042969 0.395047 -0.048122 0.006204

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 0.000012 -0.000000 0.000000 -0.000017 -0.000003 0.003788

38 H 0.000012 -0.000000 0.000000 -0.000017 -0.000003 0.003788

39 H 0.000000 0.000000 0.000000 -0.000001 0.000037 0.000063

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 0.000386 -0.005092 -0.045981 -0.000244 -0.000073 0.000008

44 H 0.000386 -0.005092 -0.045981 -0.000244 -0.000073 0.000008

45 H -0.000230 0.006116 -0.041902 -0.005504 0.000247 -0.000011

25 26 27 28 29 30

1 C -0.016064 0.009718 -0.048122 0.000000 0.000001 -0.000363

2 N 0.117187 0.009064 0.006145 0.000001 0.000078 0.000058

3 C -0.017088 -0.067920 0.009693 0.000002 -0.000073 0.000000

4 C -0.000775 0.263816 -0.042969 -0.000000 -0.000161 -0.000000

5 C -0.000617 -0.056886 0.395047 0.000000 -0.000005 -0.000039

6 N -0.005602 0.015348 -0.000010 -0.000021 0.006670 0.000000

7 C -0.016393 -0.000309 0.000010 0.009463 -0.048824 0.000000

8 N 0.117686 0.000062 0.000001 0.008839 0.006390 -0.000000

9 C -0.017072 0.000000 0.000000 -0.069055 0.009749 0.000000

10 C -0.000679 0.000000 0.000000 0.265326 -0.042812 -0.000000

11 C -0.000485 -0.000043 -0.000000 -0.055165 0.394852 -0.000000

12 N -0.005180 -0.000017 0.006204 -0.000000 0.000000 0.014189

13 C -0.000679 -0.000000 -0.000145 -0.000000 -0.000000 0.265326

14 C -0.000485 0.000000 -0.000004 -0.000000 -0.000000 -0.055165

15 C -0.016393 0.000000 0.000001 0.000000 0.000000 0.009463

16 N 0.117686 0.000001 0.000073 -0.000000 0.000000 0.008839

17 C -0.017072 0.000002 -0.000138 0.000000 -0.000000 -0.069055

18 N -0.005602 -0.000000 0.000000 0.000000 -0.000000 -0.000021

19 N 0.117187 -0.000000 0.000000 0.000058 0.000001 0.000001

20 C -0.017088 0.000000 -0.000000 0.000000 0.000000 0.000002

21 C -0.000775 -0.000000 -0.000000 -0.000000 0.000000 -0.000000

22 C -0.000617 -0.000000 -0.000000 -0.000039 -0.000000 0.000000

23 C -0.016064 0.000000 -0.000000 -0.000363 0.000011 0.000000

24 N -0.005180 0.000000 -0.000000 0.014189 -0.000007 -0.000000

25 Zn 10.217665 0.000459 -0.000072 0.000335 0.000011 0.000335

26 C 0.000459 5.365876 -0.004577 -0.000000 0.000073 -0.000000

27 H -0.000072 -0.004577 0.448546 -0.000000 -0.000000 0.000066

28 C 0.000335 -0.000000 -0.000000 5.366454 -0.004545 0.000000

29 H 0.000011 0.000073 -0.000000 -0.004545 0.450005 -0.000000

30 C 0.000335 -0.000000 0.000066 0.000000 -0.000000 5.366454

31 H 0.000011 -0.000000 -0.000000 -0.000000 0.000000 -0.004545

32 C 0.000459 0.000000 -0.000000 -0.000000 -0.000000 -0.000000

33 H -0.000072 -0.000000 0.000000 0.000066 -0.000000 -0.000000

34 H 0.000070 0.389413 0.001331 -0.000000 0.000000 -0.000000

35 H 0.000085 0.387943 -0.000123 -0.000000 0.000040 0.000000

36 H 0.000085 0.387943 -0.000123 -0.000000 0.000040 0.000000

37 H 0.000074 0.000000 0.000000 0.387391 -0.000114 0.000000

38 H 0.000074 0.000000 0.000000 0.387391 -0.000114 0.000000

39 H 0.000065 -0.000000 0.000000 0.389172 0.001353 -0.000000

40 H 0.000074 -0.000000 0.000036 0.000000 -0.000000 0.387391

41 H 0.000074 -0.000000 0.000036 0.000000 -0.000000 0.387391

42 H 0.000065 -0.000000 0.000000 -0.000000 -0.000000 0.389172

43 H 0.000085 0.000000 -0.000000 0.000000 0.000000 -0.000000

44 H 0.000085 0.000000 -0.000000 0.000000 0.000000 -0.000000

45 H 0.000070 -0.000000 -0.000000 -0.000000 0.000000 -0.000000

31 32 33 34 35 36

1 C 0.000011 0.000000 -0.000000 0.000247 -0.000073 -0.000073

2 N 0.000001 -0.000000 0.000000 -0.000230 0.000386 0.000386

3 C 0.000000 0.000000 -0.000000 0.006116 -0.005092 -0.005092

4 C 0.000000 -0.000000 -0.000000 -0.041902 -0.045981 -0.045981

5 C -0.000000 -0.000000 -0.000000 -0.005504 -0.000244 -0.000244

6 N -0.000000 -0.000000 0.000000 0.000087 0.004671 0.004671

7 C 0.000000 0.000000 0.000001 0.000039 -0.000029 -0.000029

8 N 0.000000 0.000001 0.000073 0.000000 0.000012 0.000012

9 C -0.000000 0.000002 -0.000138 0.000000 0.000000 0.000000

10 C -0.000000 -0.000000 -0.000145 0.000000 0.000000 0.000000

11 C -0.000000 0.000000 -0.000004 -0.000001 -0.000031 -0.000031

12 N -0.000007 0.000000 -0.000000 -0.000011 0.000008 0.000008

13 C -0.042812 0.000000 0.000000 0.000000 0.000000 0.000000

14 C 0.394852 -0.000043 -0.000000 0.000000 -0.000000 -0.000000

15 C -0.048824 -0.000309 0.000010 -0.000000 0.000000 0.000000

16 N 0.006390 0.000062 0.000001 -0.000000 0.000000 0.000000

17 C 0.009749 0.000000 0.000000 0.000001 -0.000000 -0.000000

18 N 0.006670 0.015348 -0.000010 -0.000000 -0.000000 -0.000000

19 N 0.000078 0.009064 0.006145 -0.000000 0.000000 0.000000

20 C -0.000073 -0.067920 0.009693 0.000000 0.000000 0.000000

21 C -0.000161 0.263816 -0.042969 0.000000 0.000000 0.000000

22 C -0.000005 -0.056886 0.395047 0.000000 -0.000000 -0.000000

23 C 0.000001 0.009718 -0.048122 0.000000 -0.000000 -0.000000

24 N 0.000000 -0.000017 0.006204 0.000000 0.000000 0.000000

25 Zn 0.000011 0.000459 -0.000072 0.000070 0.000085 0.000085

26 C -0.000000 0.000000 -0.000000 0.389413 0.387943 0.387943

27 H -0.000000 -0.000000 0.000000 0.001331 -0.000123 -0.000123

28 C -0.000000 -0.000000 0.000066 -0.000000 -0.000000 -0.000000

29 H 0.000000 -0.000000 -0.000000 0.000000 0.000040 0.000040

30 C -0.004545 -0.000000 -0.000000 -0.000000 0.000000 0.000000

31 H 0.450005 0.000073 -0.000000 0.000000 0.000000 0.000000

32 C 0.000073 5.365876 -0.004577 -0.000000 0.000000 0.000000

33 H -0.000000 -0.004577 0.448546 -0.000000 -0.000000 -0.000000

34 H 0.000000 -0.000000 -0.000000 0.460865 -0.025604 -0.025604

35 H 0.000000 0.000000 -0.000000 -0.025604 0.477162 -0.030581

36 H 0.000000 0.000000 -0.000000 -0.025604 -0.030581 0.477162

37 H -0.000000 -0.000000 0.000036 0.000000 0.000000 -0.000000

38 H -0.000000 -0.000000 0.000036 0.000000 -0.000000 0.000000

39 H -0.000000 -0.000000 0.000000 -0.000000 -0.000000 -0.000000

40 H -0.000114 0.000000 0.000000 -0.000000 0.000000 -0.000000

41 H -0.000114 0.000000 0.000000 -0.000000 -0.000000 0.000000

42 H 0.001353 -0.000000 0.000000 -0.000000 0.000000 0.000000

43 H 0.000040 0.387943 -0.000123 0.000000 -0.000000 0.000000

44 H 0.000040 0.387943 -0.000123 0.000000 0.000000 -0.000000

45 H 0.000000 0.389413 0.001331 0.000000 0.000000 0.000000

37 38 39 40 41 42

1 C -0.000000 -0.000000 -0.000000 -0.000003 -0.000003 0.000037

2 N 0.000000 0.000000 -0.000000 0.000012 0.000012 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 -0.000017 -0.000017 -0.000001

6 N 0.000007 0.000007 -0.000011 0.000000 0.000000 0.000000

7 C -0.000163 -0.000163 0.000242 0.000000 0.000000 0.000000

8 N 0.000419 0.000419 -0.000239 0.000000 0.000000 -0.000000

9 C -0.005136 -0.005136 0.006091 0.000000 0.000000 0.000000

10 C -0.043694 -0.043694 -0.041603 0.000000 0.000000 0.000000

11 C -0.000287 -0.000287 -0.005411 -0.000000 -0.000000 0.000000

12 N -0.000000 -0.000000 -0.000000 0.003788 0.003788 0.000063

13 C 0.000000 0.000000 0.000000 -0.043694 -0.043694 -0.041603

14 C -0.000000 -0.000000 0.000000 -0.000287 -0.000287 -0.005411

15 C 0.000000 0.000000 0.000000 -0.000163 -0.000163 0.000242

16 N 0.000000 0.000000 -0.000000 0.000419 0.000419 -0.000239

17 C 0.000000 0.000000 0.000000 -0.005136 -0.005136 0.006091

18 N 0.000000 0.000000 0.000000 0.000007 0.000007 -0.000011

19 N 0.000012 0.000012 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 -0.000017 -0.000017 -0.000001 -0.000000 -0.000000 0.000000

23 C -0.000003 -0.000003 0.000037 -0.000000 -0.000000 -0.000000

24 N 0.003788 0.003788 0.000063 -0.000000 -0.000000 -0.000000

25 Zn 0.000074 0.000074 0.000065 0.000074 0.000074 0.000065

26 C 0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000000

27 H 0.000000 0.000000 0.000000 0.000036 0.000036 0.000000

28 C 0.387391 0.387391 0.389172 0.000000 0.000000 -0.000000

29 H -0.000114 -0.000114 0.001353 -0.000000 -0.000000 -0.000000

30 C 0.000000 0.000000 -0.000000 0.387391 0.387391 0.389172

31 H -0.000000 -0.000000 -0.000000 -0.000114 -0.000114 0.001353

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

33 H 0.000036 0.000036 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 0.470702 -0.028289 -0.025498 0.000000 -0.000000 0.000000

38 H -0.028289 0.470702 -0.025498 -0.000000 0.000000 0.000000

39 H -0.025498 -0.025498 0.459398 0.000000 0.000000 0.000000

40 H 0.000000 -0.000000 0.000000 0.470702 -0.028289 -0.025498

41 H -0.000000 0.000000 0.000000 -0.028289 0.470702 -0.025498

42 H 0.000000 0.000000 0.000000 -0.025498 -0.025498 0.459398

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 -0.000031 -0.000031 -0.000001

15 C -0.000029 -0.000029 0.000039

16 N 0.000012 0.000012 0.000000

17 C 0.000000 0.000000 0.000000

18 N 0.004671 0.004671 0.000087

19 N 0.000386 0.000386 -0.000230

20 C -0.005092 -0.005092 0.006116

21 C -0.045981 -0.045981 -0.041902

22 C -0.000244 -0.000244 -0.005504

23 C -0.000073 -0.000073 0.000247

24 N 0.000008 0.000008 -0.000011

25 Zn 0.000085 0.000085 0.000070

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 0.000040 0.000040 0.000000

32 C 0.387943 0.387943 0.389413

33 H -0.000123 -0.000123 0.001331

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 0.477162 -0.030581 -0.025604

44 H -0.030581 0.477162 -0.025604

45 H -0.025604 -0.025604 0.460865

Atomic-Atomic Spin Densities.

1 2 3 4 5 6

1 C 0.338694 -0.025239 -0.016674 -0.021271 0.031946 0.001291

2 N -0.025239 -0.016982 0.014147 0.000689 -0.000542 -0.002722

3 C -0.016674 0.014147 0.156251 0.035686 -0.007494 -0.022454

4 C -0.021271 0.000689 0.035686 0.176267 -0.021551 -0.007208

5 C 0.031946 -0.000542 -0.007494 -0.021551 -0.061573 0.000068

6 N 0.001291 -0.002722 -0.022454 -0.007208 0.000068 0.183260

7 C 0.000085 0.000936 -0.009801 -0.000202 0.000032 -0.018318

8 N -0.000089 0.000962 0.000745 0.000029 -0.000001 -0.003523

9 C 0.000003 -0.000091 0.000085 -0.000002 0.000000 0.001164

10 C 0.000000 -0.000004 0.000047 -0.000000 -0.000000 0.000225

11 C -0.000003 0.000027 -0.000145 0.000052 -0.000000 -0.006176

12 N 0.005298 0.001239 0.000073 -0.000008 0.000607 0.000002

13 C -0.000756 0.000005 0.000002 0.000000 0.000013 -0.000000

14 C 0.000120 -0.000008 -0.000000 -0.000000 0.000000 0.000000

15 C 0.000243 -0.000004 -0.000007 -0.000000 0.000001 0.000000

16 N 0.001847 -0.000568 -0.000019 -0.000010 0.000015 0.000003

17 C -0.022914 0.001518 0.000260 0.000139 -0.000646 -0.000006

18 N -0.000005 0.000002 0.000000 0.000000 -0.000000 -0.000000

19 N 0.000012 -0.000027 -0.000005 -0.000000 0.000000 0.000002

20 C -0.000004 -0.000005 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 -0.000001 0.000012 -0.000004 0.000000 -0.000000 -0.000005

24 N 0.000000 -0.000000 -0.000000 -0.000000 0.000000 0.000002

25 Zn 0.000014 0.000304 -0.000191 -0.000054 -0.000040 0.000046

26 C -0.000128 -0.000064 -0.000562 -0.006979 0.002325 0.000322

27 H -0.000021 -0.000007 -0.000147 0.000375 0.001025 -0.000003

28 C 0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000001

29 H -0.000000 -0.000000 -0.000019 0.000001 0.000000 0.000023

30 C 0.000046 0.000001 -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 0.000009 -0.000001 0.000031 -0.000360 0.000095 -0.000008

35 H 0.000104 -0.000037 -0.000836 -0.004197 0.000272 0.000578

36 H 0.000104 -0.000037 -0.000836 -0.004197 0.000272 0.000578

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 0.000037 -0.000000 -0.000000 -0.000000 0.000003 0.000000

41 H 0.000037 -0.000000 -0.000000 -0.000000 0.000003 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 0.000085 -0.000089 0.000003 0.000000 -0.000003 0.005298

2 N 0.000936 0.000962 -0.000091 -0.000004 0.000027 0.001239

3 C -0.009801 0.000745 0.000085 0.000047 -0.000145 0.000073

4 C -0.000202 0.000029 -0.000002 -0.000000 0.000052 -0.000008

5 C 0.000032 -0.000001 0.000000 -0.000000 -0.000000 0.000607

6 N -0.018318 -0.003523 0.001164 0.000225 -0.006176 0.000002

7 C 0.153355 0.017293 -0.016317 -0.009891 0.027602 -0.000000

8 N 0.017293 -0.009297 -0.030957 -0.002554 0.002721 -0.000000

9 C -0.016317 -0.030957 0.340354 0.038639 -0.017003 0.000000

10 C -0.009891 -0.002554 0.038639 0.009808 -0.024014 0.000000

11 C 0.027602 0.002721 -0.017003 -0.024014 0.092920 -0.000000

12 N -0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.152605

13 C -0.000000 0.000000 0.000000 0.000000 0.000000 -0.000522

14 C -0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000158

15 C 0.000001 -0.000003 -0.000004 -0.000000 -0.000000 0.000208

16 N -0.000003 -0.000031 0.000011 0.000000 -0.000000 0.001605

17 C -0.000004 0.000011 -0.000000 0.000000 0.000000 0.002822

18 N 0.000000 0.000003 -0.000006 -0.000000 0.000000 0.000002

19 N -0.000004 -0.000568 0.001518 0.000005 -0.000008 -0.000000

20 C -0.000007 -0.000019 0.000260 0.000002 -0.000000 -0.000000

21 C -0.000000 -0.000010 0.000139 0.000000 -0.000000 -0.000000

22 C 0.000001 0.000015 -0.000646 0.000013 0.000000 0.000000

23 C 0.000243 0.001847 -0.022914 -0.000756 0.000120 0.000000

24 N 0.000208 0.001605 0.002822 -0.000522 -0.000158 -0.000000

25 Zn 0.000394 0.000188 -0.000602 -0.000114 0.000028 0.000027

26 C 0.000019 -0.000000 -0.000000 0.000000 -0.000002 0.000001

27 H 0.000000 -0.000000 -0.000000 -0.000000 0.000000 0.000159

28 C -0.000093 0.000070 -0.002415 -0.001553 0.001836 0.000000

29 H 0.000363 -0.000071 -0.000208 0.000478 -0.000136 -0.000000

30 C 0.000000 -0.000000 0.000000 0.000000 -0.000000 0.000509

31 H 0.000000 -0.000000 -0.000000 -0.000000 0.000000 -0.000004

32 C 0.000000 0.000000 -0.000000 -0.000000 -0.000000 0.000000

33 H -0.000000 0.000001 -0.000009 0.000000 0.000000 0.000000

34 H -0.000000 -0.000000 0.000000 -0.000000 0.000000 -0.000000

35 H -0.000004 -0.000002 0.000000 0.000000 -0.000009 0.000000

36 H -0.000004 -0.000002 0.000000 0.000000 -0.000009 0.000000

37 H 0.000016 0.000016 -0.000660 -0.000381 0.000204 0.000000

38 H 0.000016 0.000016 -0.000660 -0.000381 0.000204 0.000000

39 H 0.000020 0.000001 0.000062 -0.000152 -0.000075 -0.000000

40 H 0.000000 -0.000000 -0.000000 -0.000000 0.000000 -0.000021

41 H 0.000000 -0.000000 -0.000000 -0.000000 0.000000 -0.000021

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 -0.000756 0.000120 0.000243 0.001847 -0.022914 -0.000005

2 N 0.000005 -0.000008 -0.000004 -0.000568 0.001518 0.000002

3 C 0.000002 -0.000000 -0.000007 -0.000019 0.000260 0.000000

4 C 0.000000 -0.000000 -0.000000 -0.000010 0.000139 0.000000

5 C 0.000013 0.000000 0.000001 0.000015 -0.000646 -0.000000

6 N -0.000000 0.000000 0.000000 0.000003 -0.000006 -0.000000

7 C -0.000000 -0.000000 0.000001 -0.000003 -0.000004 0.000000

8 N 0.000000 -0.000000 -0.000003 -0.000031 0.000011 0.000003

9 C 0.000000 0.000000 -0.000004 0.000011 -0.000000 -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 -0.000522 -0.000158 0.000208 0.001605 0.002822 0.000002

13 C 0.009808 -0.024014 -0.009891 -0.002554 0.038639 0.000225

14 C -0.024014 0.092920 0.027602 0.002721 -0.017003 -0.006176

15 C -0.009891 0.027602 0.153355 0.017293 -0.016317 -0.018318

16 N -0.002554 0.002721 0.017293 -0.009297 -0.030957 -0.003523

17 C 0.038639 -0.017003 -0.016317 -0.030957 0.340354 0.001164

18 N 0.000225 -0.006176 -0.018318 -0.003523 0.001164 0.183260

19 N -0.000004 0.000027 0.000936 0.000962 -0.000091 -0.002722

20 C 0.000047 -0.000145 -0.009801 0.000745 0.000085 -0.022454

21 C -0.000000 0.000052 -0.000202 0.000029 -0.000002 -0.007208

22 C -0.000000 -0.000000 0.000032 -0.000001 0.000000 0.000068

23 C 0.000000 -0.000003 0.000085 -0.000089 0.000003 0.001291

24 N 0.000000 -0.000000 -0.000000 -0.000000 0.000000 0.000002

25 Zn -0.000114 0.000028 0.000394 0.000188 -0.000602 0.000046

26 C -0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000000

27 H 0.000000 0.000000 -0.000000 0.000001 -0.000009 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 -0.001553 0.001836 -0.000093 0.000070 -0.002415 -0.000001

31 H 0.000478 -0.000136 0.000363 -0.000071 -0.000208 0.000023

32 C 0.000000 -0.000002 0.000019 -0.000000 -0.000000 0.000322

33 H -0.000000 0.000000 0.000000 -0.000000 -0.000000 -0.000003

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 -0.000381 0.000204 0.000016 0.000016 -0.000660 -0.000000

41 H -0.000381 0.000204 0.000016 0.000016 -0.000660 -0.000000

42 H -0.000152 -0.000075 0.000020 0.000001 0.000062 -0.000000

43 H 0.000000 -0.000009 -0.000004 -0.000002 0.000000 0.000578

44 H 0.000000 -0.000009 -0.000004 -0.000002 0.000000 0.000578

45 H -0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.000008

19 20 21 22 23 24

1 C 0.000012 -0.000004 0.000000 -0.000000 -0.000001 0.000000

2 N -0.000027 -0.000005 -0.000000 0.000000 0.000012 -0.000000

3 C -0.000005 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 0.000002 0.000000 0.000000 -0.000000 -0.000005 0.000002

7 C -0.000004 -0.000007 -0.000000 0.000001 0.000243 0.000208

8 N -0.000568 -0.000019 -0.000010 0.000015 0.001847 0.001605

9 C 0.001518 0.000260 0.000139 -0.000646 -0.022914 0.002822

10 C 0.000005 0.000002 0.000000 0.000013 -0.000756 -0.000522

11 C -0.000008 -0.000000 -0.000000 0.000000 0.000120 -0.000158

12 N -0.000000 -0.000000 -0.000000 0.000000 0.000000 -0.000000

13 C -0.000004 0.000047 -0.000000 -0.000000 0.000000 0.000000

14 C 0.000027 -0.000145 0.000052 -0.000000 -0.000003 -0.000000

15 C 0.000936 -0.009801 -0.000202 0.000032 0.000085 -0.000000

16 N 0.000962 0.000745 0.000029 -0.000001 -0.000089 -0.000000

17 C -0.000091 0.000085 -0.000002 0.000000 0.000003 0.000000

18 N -0.002722 -0.022454 -0.007208 0.000068 0.001291 0.000002

19 N -0.016982 0.014147 0.000689 -0.000542 -0.025239 0.001239

20 C 0.014147 0.156251 0.035686 -0.007494 -0.016674 0.000073

21 C 0.000689 0.035686 0.176267 -0.021551 -0.021271 -0.000008

22 C -0.000542 -0.007494 -0.021551 -0.061573 0.031946 0.000607

23 C -0.025239 -0.016674 -0.021271 0.031946 0.338694 0.005298

24 N 0.001239 0.000073 -0.000008 0.000607 0.005298 -0.152605

25 Zn 0.000304 -0.000191 -0.000054 -0.000040 0.000014 0.000027

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 0.000001 -0.000000 0.000000 0.000002 0.000046 0.000509

29 H -0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000004

30 C 0.000000 0.000000 0.000000 -0.000000 0.000000 0.000000

31 H -0.000000 -0.000019 0.000001 0.000000 -0.000000 -0.000000

32 C -0.000064 -0.000562 -0.006979 0.002325 -0.000128 0.000001

33 H -0.000007 -0.000147 0.000375 0.001025 -0.000021 0.000159

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 0.000003 0.000037 -0.000021

38 H -0.000000 -0.000000 -0.000000 0.000003 0.000037 -0.000021

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 -0.000037 -0.000836 -0.004197 0.000272 0.000104 0.000000

44 H -0.000037 -0.000836 -0.004197 0.000272 0.000104 0.000000

45 H -0.000001 0.000031 -0.000360 0.000095 0.000009 -0.000000

25 26 27 28 29 30

1 C 0.000014 -0.000128 -0.000021 0.000000 -0.000000 0.000046

2 N 0.000304 -0.000064 -0.000007 0.000000 -0.000000 0.000001

3 C -0.000191 -0.000562 -0.000147 0.000000 -0.000019 -0.000000

4 C -0.000054 -0.006979 0.000375 0.000000 0.000001 0.000000

5 C -0.000040 0.002325 0.001025 -0.000000 0.000000 0.000002

6 N 0.000046 0.000322 -0.000003 -0.000001 0.000023 0.000000

7 C 0.000394 0.000019 0.000000 -0.000093 0.000363 0.000000

8 N 0.000188 -0.000000 -0.000000 0.000070 -0.000071 -0.000000

9 C -0.000602 -0.000000 -0.000000 -0.002415 -0.000208 0.000000

10 C -0.000114 0.000000 -0.000000 -0.001553 0.000478 0.000000

11 C 0.000028 -0.000002 0.000000 0.001836 -0.000136 -0.000000

12 N 0.000027 0.000001 0.000159 0.000000 -0.000000 0.000509

13 C -0.000114 -0.000000 0.000000 0.000000 -0.000000 -0.001553

14 C 0.000028 -0.000000 0.000000 -0.000000 0.000000 0.001836

15 C 0.000394 0.000000 -0.000000 0.000000 0.000000 -0.000093

16 N 0.000188 0.000000 0.000001 -0.000000 -0.000000 0.000070

17 C -0.000602 -0.000000 -0.000009 0.000000 -0.000000 -0.002415

18 N 0.000046 -0.000000 0.000000 0.000000 0.000000 -0.000001

19 N 0.000304 0.000000 -0.000000 0.000001 -0.000000 0.000000

20 C -0.000191 -0.000000 -0.000000 -0.000000 -0.000000 0.000000

21 C -0.000054 0.000000 -0.000000 0.000000 -0.000000 0.000000

22 C -0.000040 -0.000000 0.000000 0.000002 -0.000000 -0.000000

23 C 0.000014 -0.000000 0.000000 0.000046 -0.000000 0.000000

24 N 0.000027 0.000000 0.000000 0.000509 -0.000004 0.000000

25 Zn -0.000706 -0.000005 -0.000007 -0.000009 0.000006 -0.000009

26 C -0.000005 -0.013446 0.000240 0.000000 -0.000002 0.000000

27 H -0.000007 0.000240 -0.000056 -0.000000 0.000000 0.000000

28 C -0.000009 0.000000 -0.000000 -0.001029 0.000248 0.000000

29 H 0.000006 -0.000002 0.000000 0.000248 -0.005350 -0.000000

30 C -0.000009 0.000000 0.000000 0.000000 -0.000000 -0.001029

31 H 0.000006 -0.000000 0.000000 -0.000000 0.000000 0.000248

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 0.000704 -0.000032 -0.000000 -0.000000 -0.000000

35 H -0.000002 0.003103 0.000002 0.000000 -0.000001 0.000000

36 H -0.000002 0.003103 0.000002 0.000000 -0.000001 0.000000

37 H 0.000000 0.000000 0.000000 0.001115 0.000003 0.000000

38 H 0.000000 0.000000 0.000000 0.001115 0.000003 0.000000

39 H 0.000003 0.000000 -0.000000 0.000238 -0.000079 0.000000

40 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.001115

41 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.001115

42 H 0.000003 -0.000000 0.000000 0.000000 0.000000 0.000238

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 0.000009 0.000104 0.000104

2 N -0.000000 0.000000 -0.000000 -0.000001 -0.000037 -0.000037

3 C -0.000000 -0.000000 -0.000000 0.000031 -0.000836 -0.000836

4 C -0.000000 0.000000 -0.000000 -0.000360 -0.004197 -0.004197

5 C -0.000000 -0.000000 0.000000 0.000095 0.000272 0.000272

6 N 0.000000 -0.000000 0.000000 -0.000008 0.000578 0.000578

7 C 0.000000 0.000000 -0.000000 -0.000000 -0.000004 -0.000004

8 N -0.000000 0.000000 0.000001 -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 0.000000 -0.000000 0.000000 0.000000

11 C 0.000000 -0.000000 0.000000 0.000000 -0.000009 -0.000009

12 N -0.000004 0.000000 0.000000 -0.000000 0.000000 0.000000

13 C 0.000478 0.000000 -0.000000 -0.000000 -0.000000 -0.000000

14 C -0.000136 -0.000002 0.000000 -0.000000 0.000000 0.000000

15 C 0.000363 0.000019 0.000000 0.000000 0.000000 0.000000

16 N -0.000071 -0.000000 -0.000000 0.000000 0.000000 0.000000

17 C -0.000208 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000

18 N 0.000023 0.000322 -0.000003 0.000000 -0.000000 -0.000000

19 N -0.000000 -0.000064 -0.000007 -0.000000 0.000000 0.000000

20 C -0.000019 -0.000562 -0.000147 -0.000000 0.000000 0.000000

21 C 0.000001 -0.006979 0.000375 -0.000000 0.000000 0.000000

22 C 0.000000 0.002325 0.001025 0.000000 -0.000000 -0.000000

23 C -0.000000 -0.000128 -0.000021 0.000000 -0.000000 -0.000000

24 N -0.000000 0.000001 0.000159 -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 0.000704 0.003103 0.003103

27 H 0.000000 -0.000000 0.000000 -0.000032 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 0.000248 0.000000 -0.000000 -0.000000 0.000000 0.000000

31 H -0.005350 -0.000002 0.000000 -0.000000 0.000000 0.000000

32 C -0.000002 -0.013446 0.000240 -0.000000 -0.000000 -0.000000

33 H 0.000000 0.000240 -0.000056 0.000000 -0.000000 -0.000000

34 H -0.000000 -0.000000 0.000000 -0.000364 -0.000088 -0.000088

35 H 0.000000 -0.000000 -0.000000 -0.000088 0.012430 -0.003647

36 H 0.000000 -0.000000 -0.000000 -0.000088 -0.003647 0.012430

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 -0.000079 0.000000 -0.000000 -0.000000 0.000000 0.000000

43 H -0.000001 0.003103 0.000002 0.000000 -0.000000 0.000000

44 H -0.000001 0.003103 0.000002 0.000000 0.000000 -0.000000

45 H -0.000000 0.000704 -0.000032 -0.000000 0.000000 0.000000

37 38 39 40 41 42

1 C 0.000000 0.000000 0.000000 0.000037 0.000037 -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 0.000003 0.000003 0.000000

6 N -0.000000 -0.000000 -0.000000 0.000000 0.000000 0.000000

7 C 0.000016 0.000016 0.000020 0.000000 0.000000 0.000000

8 N 0.000016 0.000016 0.000001 -0.000000 -0.000000 -0.000000

9 C -0.000660 -0.000660 0.000062 -0.000000 -0.000000 -0.000000

10 C -0.000381 -0.000381 -0.000152 -0.000000 -0.000000 -0.000000

11 C 0.000204 0.000204 -0.000075 0.000000 0.000000 0.000000

12 N 0.000000 0.000000 -0.000000 -0.000021 -0.000021 -0.000002

13 C -0.000000 -0.000000 -0.000000 -0.000381 -0.000381 -0.000152

14 C 0.000000 0.000000 0.000000 0.000204 0.000204 -0.000075

15 C 0.000000 0.000000 0.000000 0.000016 0.000016 0.000020

16 N -0.000000 -0.000000 -0.000000 0.000016 0.000016 0.000001

17 C -0.000000 -0.000000 -0.000000 -0.000660 -0.000660 0.000062

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 0.000003 0.000003 0.000000 0.000000 0.000000 -0.000000

23 C 0.000037 0.000037 -0.000000 0.000000 0.000000 0.000000

24 N -0.000021 -0.000021 -0.000002 0.000000 0.000000 -0.000000

25 Zn 0.000000 0.000000 0.000003 0.000000 0.000000 0.000003

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 0.001115 0.001115 0.000238 0.000000 0.000000 0.000000

29 H 0.000003 0.000003 -0.000079 0.000000 0.000000 0.000000

30 C 0.000000 0.000000 0.000000 0.001115 0.001115 0.000238

31 H 0.000000 0.000000 0.000000 0.000003 0.000003 -0.000079

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 0.001613 -0.000189 0.000055 0.000000 -0.000000 0.000000

38 H -0.000189 0.001613 0.000055 -0.000000 0.000000 0.000000

39 H 0.000055 0.000055 -0.000662 0.000000 0.000000 0.000000

40 H 0.000000 -0.000000 0.000000 0.001613 -0.000189 0.000055

41 H -0.000000 0.000000 0.000000 -0.000189 0.001613 0.000055

42 H 0.000000 0.000000 0.000000 0.000055 0.000055 -0.000662

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 -0.000009 -0.000009 0.000000

15 C -0.000004 -0.000004 -0.000000

16 N -0.000002 -0.000002 -0.000000

17 C 0.000000 0.000000 0.000000

18 N 0.000578 0.000578 -0.000008

19 N -0.000037 -0.000037 -0.000001

20 C -0.000836 -0.000836 0.000031

21 C -0.004197 -0.004197 -0.000360

22 C 0.000272 0.000272 0.000095

23 C 0.000104 0.000104 0.000009

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 0.003103 0.003103 0.000704

33 H 0.000002 0.000002 -0.000032

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 0.012430 -0.003647 -0.000088

44 H -0.003647 0.012430 -0.000088

45 H -0.000088 -0.000088 -0.000364

Mulliken charges and spin densities:

1 2

1 C 0.382972 0.292785

2 N -0.682812 -0.026496

3 C 0.401753 0.148135

4 C 0.009274 0.147198

5 C -0.290219 -0.055168

6 N -0.463621 0.127140

7 C 0.407891 0.145938

8 N -0.685325 -0.021602

9 C 0.380639 0.292558

10 C 0.022136 0.008897

11 C -0.302824 0.077975

12 N -0.410908 -0.140788

13 C 0.022136 0.008897

14 C -0.302824 0.077975

15 C 0.407891 0.145938

16 N -0.685325 -0.021602

17 C 0.380639 0.292558

18 N -0.463621 0.127140

19 N -0.682812 -0.026496

20 C 0.401753 0.148135

21 C 0.009274 0.147198

22 C -0.290219 -0.055168

23 C 0.382972 0.292785

24 N -0.410908 -0.140788

25 Zn 1.470128 -0.000736

26 C -0.699967 -0.011371

27 H 0.229095 0.001525

28 C -0.699499 0.000078

29 H 0.227379 -0.004746

30 C -0.699499 0.000078

31 H 0.227379 -0.004746

32 C -0.699967 -0.011371

33 H 0.229095 0.001525

34 H 0.240686 -0.000103

35 H 0.237450 0.007664

36 H 0.237450 0.007664

37 H 0.240773 0.001812

38 H 0.240773 0.001812

39 H 0.241838 -0.000539

40 H 0.240773 0.001812

41 H 0.240773 0.001812

42 H 0.241838 -0.000539

43 H 0.237450 0.007664

44 H 0.237450 0.007664

45 H 0.240686 -0.000103

Sum of Mulliken charges = -0.00000 2.00000

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

1 2

1 C 0.382972 0.292785

2 N -0.682812 -0.026496

3 C 0.401753 0.148135

4 C 0.009274 0.147198

5 C -0.061125 -0.053644

6 N -0.463621 0.127140

7 C 0.407891 0.145938

8 N -0.685325 -0.021602

9 C 0.380639 0.292558

10 C 0.022136 0.008897

11 C -0.075445 0.073229

12 N -0.410908 -0.140788

13 C 0.022136 0.008897

14 C -0.075445 0.073229

15 C 0.407891 0.145938

16 N -0.685325 -0.021602

17 C 0.380639 0.292558

18 N -0.463621 0.127140

19 N -0.682812 -0.026496

20 C 0.401753 0.148135

21 C 0.009274 0.147198

22 C -0.061125 -0.053644

23 C 0.382972 0.292785

24 N -0.410908 -0.140788

25 Zn 1.470128 -0.000736

26 C 0.015619 0.003855

28 C 0.023886 0.003163

30 C 0.023886 0.003163

32 C 0.015619 0.003855

Electronic spatial extent (au): <R\*\*2>= 11239.1291

Charge= 0.0000 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= -161.8901 YY= -156.8603 ZZ= -172.0597

XY= -1.5035 XZ= 0.0000 YZ= -0.0000

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

XX= 1.7133 YY= 6.7431 ZZ= -8.4564

XY= -1.5035 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= -7062.6246 YYYY= -6923.7061 ZZZZ= -207.4954 XXXY= -292.3869

XXXZ= 0.0000 YYYX= 260.6353 YYYZ= -0.0000 ZZZX= -0.0000

ZZZY= -0.0000 XXYY= -2457.4531 XXZZ= -1363.4443 YYZZ= -1358.7158

XXYZ= -0.0000 YYXZ= -0.0000 ZZXY= -0.8985

N-N= 2.759873834275D+03 E-N=-8.571608274077D+03 KE= 1.320695961116D+03

Symmetry AG KE= 6.508408349168D+02

Symmetry BG KE= 6.704627111415D+01

Symmetry AU KE= 2.105132716833D+01

Symmetry BU KE= 5.817575279171D+02

Isotropic Fermi Contact Couplings

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

1 C(13) 0.02293 12.88951 4.59930 4.29948

2 N(14) -0.00761 -1.22943 -0.43869 -0.41009

3 C(13) 0.00192 1.07763 0.38452 0.35946

4 C(13) 0.00549 3.08803 1.10189 1.03006

5 C(13) -0.01328 -7.46298 -2.66298 -2.48938

6 N(14) 0.01115 1.80128 0.64274 0.60084

7 C(13) 0.00325 1.82458 0.65106 0.60862

8 N(14) -0.00695 -1.12340 -0.40086 -0.37472

9 C(13) 0.02157 12.12663 4.32708 4.04501

10 C(13) -0.00786 -4.42018 -1.57723 -1.47441

11 C(13) -0.00056 -0.31585 -0.11270 -0.10536

12 N(14) -0.02208 -3.56753 -1.27298 -1.19000

13 C(13) -0.00786 -4.42018 -1.57723 -1.47441

14 C(13) -0.00056 -0.31585 -0.11270 -0.10536

15 C(13) 0.00325 1.82458 0.65106 0.60862

16 N(14) -0.00695 -1.12340 -0.40086 -0.37472

17 C(13) 0.02157 12.12663 4.32708 4.04501

18 N(14) 0.01115 1.80128 0.64274 0.60084

19 N(14) -0.00761 -1.22943 -0.43869 -0.41009

20 C(13) 0.00192 1.07763 0.38452 0.35946

21 C(13) 0.00549 3.08803 1.10189 1.03006

22 C(13) -0.01328 -7.46298 -2.66298 -2.48938

23 C(13) 0.02293 12.88951 4.59930 4.29948

24 N(14) -0.02208 -3.56753 -1.27298 -1.19000

25 Zn(67) -0.00000 -0.00000 -0.00000 -0.00000

26 C(13) -0.00531 -2.98535 -1.06525 -0.99581

27 H(1) 0.00026 0.57288 0.20442 0.19109

28 C(13) -0.00127 -0.71598 -0.25548 -0.23883

29 H(1) -0.00148 -3.30983 -1.18103 -1.10404

30 C(13) -0.00127 -0.71598 -0.25548 -0.23883

31 H(1) -0.00148 -3.30983 -1.18103 -1.10404

32 C(13) -0.00531 -2.98535 -1.06525 -0.99581

33 H(1) 0.00026 0.57288 0.20442 0.19109

34 H(1) -0.00002 -0.03941 -0.01406 -0.01315

35 H(1) 0.00406 9.08247 3.24085 3.02959

36 H(1) 0.00406 9.08247 3.24085 3.02959

37 H(1) 0.00141 3.14791 1.12325 1.05003

38 H(1) 0.00141 3.14791 1.12325 1.05003

39 H(1) -0.00019 -0.42501 -0.15165 -0.14177

40 H(1) 0.00141 3.14791 1.12325 1.05003

41 H(1) 0.00141 3.14791 1.12325 1.05003

42 H(1) -0.00019 -0.42501 -0.15165 -0.14177

43 H(1) 0.00406 9.08247 3.24085 3.02959

44 H(1) 0.00406 9.08247 3.24085 3.02959

45 H(1) -0.00002 -0.03941 -0.01406 -0.01315

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

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

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

1 Atom -0.178871 -0.185806 0.364677

2 Atom 0.005795 0.008115 -0.013910

3 Atom -0.101272 -0.085949 0.187221

4 Atom -0.086625 -0.094447 0.181071

5 Atom 0.017802 0.020502 -0.038304

6 Atom -0.191506 -0.180600 0.372106

7 Atom -0.090053 -0.091649 0.181702

8 Atom 0.004238 -0.001629 -0.002609

9 Atom -0.185953 -0.181482 0.367435

10 Atom -0.019664 -0.013551 0.033215

11 Atom -0.048691 -0.047153 0.095845

12 Atom 0.135795 0.116871 -0.252666

13 Atom -0.019664 -0.013551 0.033215

14 Atom -0.048691 -0.047153 0.095845

15 Atom -0.090053 -0.091649 0.181702

16 Atom 0.004238 -0.001629 -0.002609

17 Atom -0.185953 -0.181482 0.367435

18 Atom -0.191506 -0.180600 0.372106

19 Atom 0.005795 0.008115 -0.013910

20 Atom -0.101272 -0.085949 0.187221

21 Atom -0.086625 -0.094447 0.181071

22 Atom 0.017802 0.020502 -0.038304

23 Atom -0.178871 -0.185806 0.364677

24 Atom 0.135795 0.116871 -0.252666

25 Atom 0.008401 -0.004852 -0.003548

26 Atom 0.003525 -0.005494 0.001969

27 Atom 0.003870 -0.000146 -0.003724

28 Atom -0.004491 0.002875 0.001616

29 Atom 0.002239 0.001687 -0.003926

30 Atom -0.004491 0.002875 0.001616

31 Atom 0.002239 0.001687 -0.003926

32 Atom 0.003525 -0.005494 0.001969

33 Atom 0.003870 -0.000146 -0.003724

34 Atom 0.003888 -0.001588 -0.002300

35 Atom 0.004470 -0.001818 -0.002652

36 Atom 0.004470 -0.001818 -0.002652

37 Atom -0.001500 0.003484 -0.001984

38 Atom -0.001500 0.003484 -0.001984

39 Atom -0.001186 0.003142 -0.001956

40 Atom -0.001500 0.003484 -0.001984

41 Atom -0.001500 0.003484 -0.001984

42 Atom -0.001186 0.003142 -0.001956

43 Atom 0.004470 -0.001818 -0.002652

44 Atom 0.004470 -0.001818 -0.002652

45 Atom 0.003888 -0.001588 -0.002300

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XY XZ YZ

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

1 Atom -0.001207 -0.000000 0.000000

2 Atom 0.003363 -0.000000 -0.000000

3 Atom -0.001277 -0.000000 0.000000

4 Atom -0.002269 0.000000 -0.000000

5 Atom -0.001258 0.000000 -0.000000

6 Atom -0.005902 0.000000 0.000000

7 Atom -0.008021 -0.000000 0.000000

8 Atom -0.001564 -0.000000 -0.000000

9 Atom 0.004738 -0.000000 -0.000000

10 Atom -0.000020 -0.000000 -0.000000

11 Atom 0.002773 0.000000 -0.000000

12 Atom 0.009844 -0.000000 -0.000000

13 Atom -0.000020 -0.000000 -0.000000

14 Atom 0.002773 -0.000000 -0.000000

15 Atom -0.008021 0.000000 -0.000000

16 Atom -0.001564 -0.000000 0.000000

17 Atom 0.004738 -0.000000 0.000000

18 Atom -0.005902 0.000000 -0.000000

19 Atom 0.003363 0.000000 -0.000000

20 Atom -0.001277 -0.000000 -0.000000

21 Atom -0.002269 0.000000 0.000000

22 Atom -0.001258 0.000000 0.000000

23 Atom -0.001207 0.000000 0.000000

24 Atom 0.009844 0.000000 -0.000000

25 Atom 0.008147 -0.000000 -0.000000

26 Atom -0.000984 -0.000000 0.000000

27 Atom -0.002679 -0.000000 -0.000000

28 Atom 0.000318 0.000000 0.000000

29 Atom 0.008874 -0.000000 -0.000000

30 Atom 0.000318 0.000000 0.000000

31 Atom 0.008874 -0.000000 -0.000000

32 Atom -0.000984 0.000000 0.000000

33 Atom -0.002679 0.000000 0.000000

34 Atom -0.002047 0.000000 0.000000

35 Atom 0.000836 -0.002309 -0.000914

36 Atom 0.000836 0.002309 0.000914

37 Atom -0.001109 0.000858 -0.001527

38 Atom -0.001109 -0.000858 0.001527

39 Atom 0.000819 -0.000000 -0.000000

40 Atom -0.001109 -0.000858 0.001527

41 Atom -0.001109 0.000858 -0.001527

42 Atom 0.000819 -0.000000 0.000000

43 Atom 0.000836 0.002309 0.000914

44 Atom 0.000836 -0.002309 -0.000914

45 Atom -0.002047 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 -0.1860 -24.961 -8.907 -8.326 0.1667 0.9860 -0.0000

1 C(13) Bbb -0.1787 -23.975 -8.555 -7.997 0.9860 -0.1667 0.0000

Bcc 0.3647 48.936 17.462 16.323 0.0000 0.0000 1.0000

Baa -0.0139 -0.536 -0.191 -0.179 0.0000 0.0000 1.0000

2 N(14) Bbb 0.0034 0.131 0.047 0.044 0.8143 -0.5805 0.0000

Bcc 0.0105 0.405 0.145 0.135 0.5805 0.8143 -0.0000

Baa -0.1014 -13.604 -4.854 -4.538 0.9966 0.0825 0.0000

3 C(13) Bbb -0.0858 -11.519 -4.110 -3.842 -0.0825 0.9966 -0.0000

Bcc 0.1872 25.123 8.965 8.380 0.0000 0.0000 1.0000

Baa -0.0951 -12.756 -4.552 -4.255 0.2599 0.9656 -0.0000

4 C(13) Bbb -0.0860 -11.542 -4.119 -3.850 0.9656 -0.2599 0.0000

Bcc 0.1811 24.298 8.670 8.105 0.0000 0.0000 1.0000

Baa -0.0383 -5.140 -1.834 -1.715 0.0000 0.0000 1.0000

5 C(13) Bbb 0.0173 2.322 0.829 0.775 0.9305 0.3662 -0.0000

Bcc 0.0210 2.818 1.005 0.940 -0.3662 0.9305 -0.0000

Baa -0.1941 -7.486 -2.671 -2.497 0.9161 0.4009 -0.0000

6 N(14) Bbb -0.1780 -6.866 -2.450 -2.290 -0.4009 0.9161 -0.0000

Bcc 0.3721 14.351 5.121 4.787 0.0000 0.0000 1.0000

Baa -0.0989 -13.273 -4.736 -4.427 0.6712 0.7413 0.0000

7 C(13) Bbb -0.0828 -11.110 -3.964 -3.706 0.7413 -0.6712 -0.0000

Bcc 0.1817 24.383 8.700 8.133 0.0000 0.0000 1.0000

Baa -0.0026 -0.101 -0.036 -0.034 0.0000 0.0000 1.0000

8 N(14) Bbb -0.0020 -0.078 -0.028 -0.026 0.2425 0.9701 -0.0000

Bcc 0.0046 0.179 0.064 0.060 0.9701 -0.2425 -0.0000

Baa -0.1890 -25.356 -9.048 -8.458 0.8446 -0.5354 0.0000

9 C(13) Bbb -0.1785 -23.950 -8.546 -7.989 0.5354 0.8446 0.0000

Bcc 0.3674 49.306 17.594 16.447 0.0000 0.0000 1.0000

Baa -0.0197 -2.639 -0.942 -0.880 1.0000 0.0033 -0.0000

10 C(13) Bbb -0.0136 -1.818 -0.649 -0.607 -0.0033 1.0000 -0.0000

Bcc 0.0332 4.457 1.590 1.487 0.0000 0.0000 1.0000

Baa -0.0508 -6.817 -2.432 -2.274 0.7960 -0.6053 0.0000

11 C(13) Bbb -0.0450 -6.045 -2.157 -2.016 0.6053 0.7960 -0.0000

Bcc 0.0958 12.861 4.589 4.290 0.0000 0.0000 1.0000

Baa -0.2527 -9.745 -3.477 -3.251 0.0000 0.0000 1.0000

12 N(14) Bbb 0.1127 4.346 1.551 1.450 -0.3918 0.9201 -0.0000

Bcc 0.1400 5.399 1.926 1.801 0.9201 0.3918 -0.0000

Baa -0.0197 -2.639 -0.942 -0.880 1.0000 0.0033 -0.0000

13 C(13) Bbb -0.0136 -1.818 -0.649 -0.607 -0.0033 1.0000 -0.0000

Bcc 0.0332 4.457 1.590 1.487 0.0000 0.0000 1.0000

Baa -0.0508 -6.817 -2.432 -2.274 0.7960 -0.6053 -0.0000

14 C(13) Bbb -0.0450 -6.045 -2.157 -2.016 0.6053 0.7960 -0.0000

Bcc 0.0958 12.861 4.589 4.290 0.0000 0.0000 1.0000

Baa -0.0989 -13.273 -4.736 -4.427 0.6712 0.7413 -0.0000

15 C(13) Bbb -0.0828 -11.110 -3.964 -3.706 0.7413 -0.6712 0.0000

Bcc 0.1817 24.383 8.700 8.133 0.0000 0.0000 1.0000

Baa -0.0026 -0.101 -0.036 -0.034 0.0000 0.0000 1.0000

16 N(14) Bbb -0.0020 -0.078 -0.028 -0.026 0.2425 0.9701 -0.0000

Bcc 0.0046 0.179 0.064 0.060 0.9701 -0.2425 0.0000

Baa -0.1890 -25.356 -9.048 -8.458 0.8446 -0.5354 0.0000

17 C(13) Bbb -0.1785 -23.950 -8.546 -7.989 0.5354 0.8446 0.0000

Bcc 0.3674 49.306 17.594 16.447 0.0000 0.0000 1.0000

Baa -0.1941 -7.486 -2.671 -2.497 0.9161 0.4009 0.0000

18 N(14) Bbb -0.1780 -6.866 -2.450 -2.290 -0.4009 0.9161 -0.0000

Bcc 0.3721 14.351 5.121 4.787 0.0000 0.0000 1.0000

Baa -0.0139 -0.536 -0.191 -0.179 0.0000 0.0000 1.0000

19 N(14) Bbb 0.0034 0.131 0.047 0.044 0.8143 -0.5805 -0.0000

Bcc 0.0105 0.405 0.145 0.135 0.5805 0.8143 0.0000

Baa -0.1014 -13.604 -4.854 -4.538 0.9966 0.0825 -0.0000

20 C(13) Bbb -0.0858 -11.519 -4.110 -3.842 -0.0825 0.9966 0.0000

Bcc 0.1872 25.123 8.965 8.380 0.0000 0.0000 1.0000

Baa -0.0951 -12.756 -4.552 -4.255 0.2599 0.9656 -0.0000

21 C(13) Bbb -0.0860 -11.542 -4.119 -3.850 0.9656 -0.2599 -0.0000

Bcc 0.1811 24.298 8.670 8.105 0.0000 0.0000 1.0000

Baa -0.0383 -5.140 -1.834 -1.715 0.0000 0.0000 1.0000

22 C(13) Bbb 0.0173 2.322 0.829 0.775 0.9305 0.3662 -0.0000

Bcc 0.0210 2.818 1.005 0.940 -0.3662 0.9305 0.0000

Baa -0.1860 -24.961 -8.907 -8.326 0.1667 0.9860 -0.0000

23 C(13) Bbb -0.1787 -23.975 -8.555 -7.997 0.9860 -0.1667 -0.0000

Bcc 0.3647 48.936 17.462 16.323 0.0000 0.0000 1.0000

Baa -0.2527 -9.745 -3.477 -3.251 0.0000 0.0000 1.0000

24 N(14) Bbb 0.1127 4.346 1.551 1.450 -0.3918 0.9201 -0.0000

Bcc 0.1400 5.399 1.926 1.801 0.9201 0.3918 0.0000

Baa -0.0087 -0.292 -0.104 -0.097 -0.4295 0.9031 0.0000

25 Zn(67) Bbb -0.0035 -0.119 -0.042 -0.040 0.0000 0.0000 1.0000

Bcc 0.0123 0.411 0.147 0.137 0.9031 0.4295 -0.0000

Baa -0.0056 -0.751 -0.268 -0.251 0.1072 0.9942 -0.0000

26 C(13) Bbb 0.0020 0.264 0.094 0.088 0.0000 0.0000 1.0000

Bcc 0.0036 0.487 0.174 0.163 0.9942 -0.1072 -0.0000

Baa -0.0037 -1.987 -0.709 -0.663 0.0000 0.0000 1.0000

27 H(1) Bbb -0.0015 -0.793 -0.283 -0.264 0.4473 0.8944 -0.0000

Bcc 0.0052 2.780 0.992 0.927 0.8944 -0.4473 -0.0000

Baa -0.0045 -0.604 -0.216 -0.202 0.9991 -0.0431 -0.0000

28 C(13) Bbb 0.0016 0.217 0.077 0.072 0.0000 0.0000 1.0000

Bcc 0.0029 0.388 0.138 0.129 0.0431 0.9991 -0.0000

Baa -0.0069 -3.689 -1.316 -1.231 -0.6960 0.7180 0.0000

29 H(1) Bbb -0.0039 -2.095 -0.748 -0.699 0.0000 0.0000 1.0000

Bcc 0.0108 5.784 2.064 1.929 0.7180 0.6960 -0.0000

Baa -0.0045 -0.604 -0.216 -0.202 0.9991 -0.0431 -0.0000

30 C(13) Bbb 0.0016 0.217 0.077 0.072 0.0000 0.0000 1.0000

Bcc 0.0029 0.388 0.138 0.129 0.0431 0.9991 -0.0000

Baa -0.0069 -3.689 -1.316 -1.231 -0.6960 0.7180 0.0000

31 H(1) Bbb -0.0039 -2.095 -0.748 -0.699 0.0000 0.0000 1.0000

Bcc 0.0108 5.784 2.064 1.929 0.7180 0.6960 -0.0000

Baa -0.0056 -0.751 -0.268 -0.251 0.1072 0.9942 -0.0000

32 C(13) Bbb 0.0020 0.264 0.094 0.088 -0.0000 0.0000 1.0000

Bcc 0.0036 0.487 0.174 0.163 0.9942 -0.1072 0.0000

Baa -0.0037 -1.987 -0.709 -0.663 0.0000 0.0000 1.0000

33 H(1) Bbb -0.0015 -0.793 -0.283 -0.264 0.4473 0.8944 -0.0000

Bcc 0.0052 2.780 0.992 0.927 0.8944 -0.4473 -0.0000

Baa -0.0023 -1.227 -0.438 -0.409 0.0000 0.0000 1.0000

34 H(1) Bbb -0.0023 -1.210 -0.432 -0.404 0.3156 0.9489 0.0000

Bcc 0.0046 2.438 0.870 0.813 0.9489 -0.3156 -0.0000

Baa -0.0036 -1.913 -0.683 -0.638 0.2218 0.3630 0.9050

35 H(1) Bbb -0.0017 -0.922 -0.329 -0.307 -0.2397 0.9199 -0.3103

Bcc 0.0053 2.834 1.011 0.945 0.9452 0.1481 -0.2910

Baa -0.0036 -1.913 -0.683 -0.638 -0.2218 -0.3630 0.9050

36 H(1) Bbb -0.0017 -0.922 -0.329 -0.307 -0.2397 0.9199 0.3103

Bcc 0.0053 2.834 1.011 0.945 0.9452 0.1481 0.2910

Baa -0.0027 -1.441 -0.514 -0.481 -0.4994 0.1223 0.8577

37 H(1) Bbb -0.0015 -0.787 -0.281 -0.263 0.8371 0.3231 0.4414

Bcc 0.0042 2.229 0.795 0.743 -0.2232 0.9384 -0.2637

Baa -0.0027 -1.441 -0.514 -0.481 0.4994 -0.1223 0.8577

38 H(1) Bbb -0.0015 -0.787 -0.281 -0.263 0.8371 0.3231 -0.4414

Bcc 0.0042 2.229 0.795 0.743 -0.2232 0.9384 0.2637

Baa -0.0020 -1.044 -0.372 -0.348 0.0000 0.0000 1.0000

39 H(1) Bbb -0.0013 -0.713 -0.254 -0.238 0.9837 -0.1799 0.0000

Bcc 0.0033 1.756 0.627 0.586 0.1799 0.9837 -0.0000

Baa -0.0027 -1.441 -0.514 -0.481 0.4994 -0.1223 0.8577

40 H(1) Bbb -0.0015 -0.787 -0.281 -0.263 0.8371 0.3231 -0.4414

Bcc 0.0042 2.229 0.795 0.743 -0.2232 0.9384 0.2637

Baa -0.0027 -1.441 -0.514 -0.481 -0.4994 0.1223 0.8577

41 H(1) Bbb -0.0015 -0.787 -0.281 -0.263 0.8371 0.3231 0.4414

Bcc 0.0042 2.229 0.795 0.743 -0.2232 0.9384 -0.2637

Baa -0.0020 -1.044 -0.372 -0.348 0.0000 0.0000 1.0000

42 H(1) Bbb -0.0013 -0.713 -0.254 -0.238 0.9837 -0.1799 0.0000

Bcc 0.0033 1.756 0.627 0.586 0.1799 0.9837 -0.0000

Baa -0.0036 -1.913 -0.683 -0.638 -0.2218 -0.3630 0.9050

43 H(1) Bbb -0.0017 -0.922 -0.329 -0.307 -0.2397 0.9199 0.3103

Bcc 0.0053 2.834 1.011 0.945 0.9452 0.1481 0.2910

Baa -0.0036 -1.913 -0.683 -0.638 0.2218 0.3630 0.9050

44 H(1) Bbb -0.0017 -0.922 -0.329 -0.307 -0.2397 0.9199 -0.3103

Bcc 0.0053 2.834 1.011 0.945 0.9452 0.1481 -0.2910

Baa -0.0023 -1.227 -0.438 -0.409 0.0000 0.0000 1.0000

45 H(1) Bbb -0.0023 -1.210 -0.432 -0.404 0.3156 0.9489 0.0000

Bcc 0.0046 2.438 0.870 0.813 0.9489 -0.3156 -0.0000

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

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Tue Sep 17 13:50:41 2019, MaxMem= 2415919104 cpu: 28.7

(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 13:50:45 2019, MaxMem= 2415919104 cpu: 79.0

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 13:50:45 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 13:50:56 2019, MaxMem= 2415919104 cpu: 197.2

(Enter /home/blab/g09/l716.exe)

Dipole =-7.63833441D-14-1.79412041D-13-2.22044605D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.013206312 -0.000987873 0.000000000

2 7 0.014066052 -0.007072995 -0.000000000

3 6 -0.001650060 0.016832969 -0.000000000

4 6 -0.009117488 -0.002294457 0.000000000

5 6 0.003764987 -0.000972811 0.000000000

6 7 0.003648067 -0.010537521 0.000000000

7 6 -0.007029365 0.011274170 0.000000000

8 7 -0.004468868 -0.013528589 -0.000000000

9 6 0.005047893 0.012288133 0.000000000

10 6 0.000629960 -0.005791220 -0.000000000

11 6 0.005677324 0.005528764 0.000000000

12 7 0.000366680 0.002402999 0.000000000

13 6 -0.000629960 0.005791220 -0.000000000

14 6 -0.005677324 -0.005528764 0.000000000

15 6 0.007029365 -0.011274170 -0.000000000

16 7 0.004468868 0.013528589 0.000000000

17 6 -0.005047893 -0.012288133 -0.000000000

18 7 -0.003648067 0.010537521 -0.000000000

19 7 -0.014066052 0.007072995 0.000000000

20 6 0.001650060 -0.016832969 0.000000000

21 6 0.009117488 0.002294457 -0.000000000

22 6 -0.003764987 0.000972811 0.000000000

23 6 0.013206312 0.000987873 -0.000000000

24 7 -0.000366680 -0.002402999 0.000000000

25 30 0.000000000 -0.000000000 -0.000000000

26 6 0.000868643 0.001353189 -0.000000000

27 1 0.000837096 0.000604829 -0.000000000

28 6 -0.000657984 0.000494932 0.000000000

29 1 -0.000794367 0.000884939 -0.000000000

30 6 0.000657984 -0.000494932 -0.000000000

31 1 0.000794367 -0.000884939 0.000000000

32 6 -0.000868643 -0.001353189 -0.000000000

33 1 -0.000837096 -0.000604829 0.000000000

34 1 0.001307277 0.000544870 0.000000000

35 1 -0.000915715 0.000355978 -0.002975482

36 1 -0.000915715 0.000355978 0.002975482

37 1 -0.000525612 -0.001178483 -0.003122029

38 1 -0.000525612 -0.001178483 0.003122029

39 1 -0.000539941 0.001354498 -0.000000000

40 1 0.000525612 0.001178483 -0.003122029

41 1 0.000525612 0.001178483 0.003122029

42 1 0.000539941 -0.001354498 -0.000000000

43 1 0.000915715 -0.000355978 -0.002975482

44 1 0.000915715 -0.000355978 0.002975482

45 1 -0.001307277 -0.000544870 -0.000000000

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

Cartesian Forces: Max 0.016832969 RMS 0.004941391

Leave Link 716 at Tue Sep 17 13:50:57 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 0.010416657 RMS 0.002164594

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= 23.84 degrees.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.00959809 RMS(Int)= 0.00003590

Iteration 2 RMS(Cart)= 0.00007666 RMS(Int)= 0.00001084

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001084

ITry= 1 IFail=0 DXMaxC= 4.70D-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 0.01042 0.00000 0.02116 0.02115 2.59838

R2 2.76294 -0.00256 0.00000 -0.00627 -0.00628 2.75666

R3 2.53844 -0.00304 0.00000 -0.00603 -0.00602 2.53243

R4 2.57400 -0.00927 0.00000 -0.01757 -0.01756 2.55644

R5 3.79361 -0.00139 0.00000 -0.00610 -0.00614 3.78748

R6 2.79211 0.00501 0.00000 0.01284 0.01285 2.80495

R7 2.53307 0.00398 0.00000 0.00642 0.00645 2.53952

R8 2.58757 -0.00466 0.00000 -0.01005 -0.01004 2.57752

R9 2.81859 -0.00236 0.00000 -0.00710 -0.00710 2.81149

R10 2.04583 -0.00104 0.00000 -0.00290 -0.00290 2.04292

R11 2.53844 0.00423 0.00000 0.00703 0.00706 2.54550

R12 2.57723 -0.00716 0.00000 -0.01325 -0.01326 2.56397

R13 2.76294 0.00407 0.00000 0.00967 0.00967 2.77261

R14 2.57400 0.00852 0.00000 0.01724 0.01724 2.59124

R15 3.79361 -0.00144 0.00000 -0.00650 -0.00653 3.78708

R16 2.79211 -0.00027 0.00000 -0.00023 -0.00023 2.79188

R17 2.53307 -0.00472 0.00000 -0.00901 -0.00899 2.52408

R18 2.58757 -0.00541 0.00000 -0.01169 -0.01168 2.57588

R19 2.81859 -0.00227 0.00000 -0.00681 -0.00681 2.81178

R20 2.04583 -0.00117 0.00000 -0.00329 -0.00329 2.04254

R21 2.53307 -0.00472 0.00000 -0.00901 -0.00899 2.52408

R22 2.58757 -0.00541 0.00000 -0.01169 -0.01168 2.57588

R23 2.79211 -0.00027 0.00000 -0.00023 -0.00023 2.79188

R24 2.81859 -0.00227 0.00000 -0.00681 -0.00681 2.81178

R25 2.76294 0.00407 0.00000 0.00967 0.00967 2.77261

R26 2.04583 -0.00117 0.00000 -0.00329 -0.00329 2.04254

R27 2.57723 -0.00716 0.00000 -0.01325 -0.01326 2.56397

R28 2.53844 0.00423 0.00000 0.00703 0.00706 2.54550

R29 2.57400 0.00852 0.00000 0.01724 0.01724 2.59124

R30 3.79361 -0.00144 0.00000 -0.00650 -0.00653 3.78708

R31 2.53307 0.00398 0.00000 0.00642 0.00645 2.53952

R32 2.57400 -0.00927 0.00000 -0.01757 -0.01756 2.55644

R33 2.57723 0.01042 0.00000 0.02116 0.02115 2.59838

R34 3.79361 -0.00139 0.00000 -0.00610 -0.00614 3.78748

R35 2.79211 0.00501 0.00000 0.01284 0.01285 2.80495

R36 2.58757 -0.00466 0.00000 -0.01005 -0.01004 2.57752

R37 2.81859 -0.00236 0.00000 -0.00710 -0.00710 2.81149

R38 2.76294 -0.00256 0.00000 -0.00627 -0.00628 2.75666

R39 2.04583 -0.00104 0.00000 -0.00290 -0.00290 2.04292

R40 2.53844 -0.00304 0.00000 -0.00603 -0.00602 2.53243

R41 2.06599 -0.00138 0.00000 -0.00402 -0.00402 2.06197

R42 2.07798 -0.00296 0.00000 -0.00879 -0.00879 2.06919

R43 2.07798 -0.00296 0.00000 -0.00879 -0.00879 2.06919

R44 2.07798 -0.00326 0.00000 -0.00968 -0.00968 2.06830

R45 2.07798 -0.00326 0.00000 -0.00968 -0.00968 2.06830

R46 2.06599 -0.00142 0.00000 -0.00412 -0.00412 2.06187

R47 2.07798 -0.00326 0.00000 -0.00968 -0.00968 2.06830

R48 2.07798 -0.00326 0.00000 -0.00968 -0.00968 2.06830

R49 2.06599 -0.00142 0.00000 -0.00412 -0.00412 2.06187

R50 2.07798 -0.00296 0.00000 -0.00879 -0.00879 2.06919

R51 2.07798 -0.00296 0.00000 -0.00879 -0.00879 2.06919

R52 2.06599 -0.00138 0.00000 -0.00402 -0.00402 2.06197

A1 1.89137 -0.00157 0.00000 -0.00271 -0.00272 1.88865

A2 2.21236 0.00080 0.00000 0.00260 0.00259 2.21494

A3 2.17945 0.00077 0.00000 0.00011 0.00013 2.17959

A4 1.90638 0.00096 0.00000 0.00403 0.00405 1.91043

A5 2.19032 -0.00073 0.00000 -0.00176 -0.00177 2.18855

A6 2.18649 -0.00023 0.00000 -0.00227 -0.00228 2.18421

A7 1.89647 -0.00175 0.00000 -0.00769 -0.00771 1.88876

A8 2.21943 0.00390 0.00000 0.01657 0.01659 2.23601

A9 2.16729 -0.00215 0.00000 -0.00888 -0.00888 2.15841

A10 1.85108 0.00291 0.00000 0.00878 0.00878 1.85986

A11 2.17776 -0.00355 0.00000 -0.01279 -0.01279 2.16497

A12 2.25435 0.00065 0.00000 0.00401 0.00401 2.25836

A13 1.87948 -0.00054 0.00000 -0.00240 -0.00241 1.87707

A14 2.17828 0.00019 0.00000 0.00068 0.00068 2.17897

A15 2.22542 0.00035 0.00000 0.00172 0.00172 2.22715

A16 2.18698 -0.00597 0.00000 -0.02364 -0.02359 2.16339

A17 2.21236 0.00197 0.00000 0.00941 0.00942 2.22178

A18 2.17945 -0.00102 0.00000 -0.00480 -0.00480 2.17466

A19 1.89137 -0.00094 0.00000 -0.00461 -0.00463 1.88675

A20 1.90638 0.00066 0.00000 0.00311 0.00313 1.90951

A21 2.19032 0.00058 0.00000 0.00213 0.00211 2.19243

A22 2.18649 -0.00124 0.00000 -0.00524 -0.00524 2.18125

A23 1.89647 -0.00213 0.00000 -0.00486 -0.00487 1.89160

A24 2.21943 0.00261 0.00000 0.00924 0.00923 2.22866

A25 2.16729 -0.00049 0.00000 -0.00438 -0.00436 2.16292

A26 1.85108 0.00023 0.00000 0.00015 0.00015 1.85123

A27 2.17776 -0.00104 0.00000 -0.00376 -0.00376 2.17400

A28 2.25435 0.00081 0.00000 0.00361 0.00361 2.25796

A29 1.87948 0.00218 0.00000 0.00621 0.00621 1.88569

A30 2.17828 -0.00132 0.00000 -0.00452 -0.00452 2.17376

A31 2.22542 -0.00086 0.00000 -0.00169 -0.00169 2.22373

A32 2.18698 -0.00169 0.00000 -0.00704 -0.00705 2.17993

A33 1.85108 0.00023 0.00000 0.00015 0.00015 1.85123

A34 2.25435 0.00081 0.00000 0.00361 0.00361 2.25796

A35 2.17776 -0.00104 0.00000 -0.00376 -0.00376 2.17400

A36 1.87948 0.00218 0.00000 0.00621 0.00621 1.88569

A37 2.22542 -0.00086 0.00000 -0.00169 -0.00169 2.22373

A38 2.17828 -0.00132 0.00000 -0.00452 -0.00452 2.17376

A39 1.89137 -0.00094 0.00000 -0.00461 -0.00463 1.88675

A40 2.17945 -0.00102 0.00000 -0.00480 -0.00480 2.17466

A41 2.21236 0.00197 0.00000 0.00941 0.00942 2.22178

A42 1.90638 0.00066 0.00000 0.00311 0.00313 1.90951

A43 2.19032 0.00058 0.00000 0.00213 0.00211 2.19243

A44 2.18649 -0.00124 0.00000 -0.00524 -0.00524 2.18125

A45 2.16729 -0.00049 0.00000 -0.00438 -0.00436 2.16292

A46 2.21943 0.00261 0.00000 0.00924 0.00923 2.22866

A47 1.89647 -0.00213 0.00000 -0.00486 -0.00487 1.89160

A48 2.18698 -0.00597 0.00000 -0.02364 -0.02359 2.16339

A49 1.90638 0.00096 0.00000 0.00403 0.00405 1.91043

A50 2.18649 -0.00023 0.00000 -0.00227 -0.00228 2.18421

A51 2.19032 -0.00073 0.00000 -0.00176 -0.00177 2.18855

A52 2.21943 0.00390 0.00000 0.01657 0.01659 2.23601

A53 2.16729 -0.00215 0.00000 -0.00888 -0.00888 2.15841

A54 1.89647 -0.00175 0.00000 -0.00769 -0.00771 1.88876

A55 1.85108 0.00291 0.00000 0.00878 0.00878 1.85986

A56 2.17776 -0.00355 0.00000 -0.01279 -0.01279 2.16497

A57 2.25435 0.00065 0.00000 0.00401 0.00401 2.25836

A58 1.87948 -0.00054 0.00000 -0.00240 -0.00241 1.87707

A59 2.22542 0.00035 0.00000 0.00172 0.00172 2.22715

A60 2.17828 0.00019 0.00000 0.00068 0.00068 2.17897

A61 1.89137 -0.00157 0.00000 -0.00271 -0.00272 1.88865

A62 2.21236 0.00080 0.00000 0.00260 0.00259 2.21494

A63 2.17945 0.00077 0.00000 0.00011 0.00013 2.17959

A64 2.18698 -0.00169 0.00000 -0.00704 -0.00705 2.17993

A65 1.57080 -0.00025 0.00000 -0.00221 -0.00224 1.56856

A66 1.57080 0.00025 0.00000 0.00221 0.00224 1.57304

A67 1.57080 0.00025 0.00000 0.00221 0.00224 1.57304

A68 1.57080 -0.00025 0.00000 -0.00221 -0.00224 1.56856

A69 1.93538 0.00063 0.00000 0.00618 0.00617 1.94154

A70 1.93656 0.00036 0.00000 0.00115 0.00114 1.93770

A71 1.93656 0.00036 0.00000 0.00115 0.00114 1.93770

A72 1.89112 -0.00016 0.00000 0.00107 0.00106 1.89217

A73 1.89112 -0.00016 0.00000 0.00107 0.00106 1.89217

A74 1.87099 -0.00111 0.00000 -0.01119 -0.01119 1.85980

A75 1.93656 0.00019 0.00000 0.00014 0.00013 1.93669

A76 1.93656 0.00019 0.00000 0.00014 0.00013 1.93669

A77 1.93538 0.00073 0.00000 0.00666 0.00664 1.94202

A78 1.87099 -0.00090 0.00000 -0.00966 -0.00967 1.86132

A79 1.89112 -0.00014 0.00000 0.00112 0.00111 1.89223

A80 1.89112 -0.00014 0.00000 0.00112 0.00111 1.89223

A81 1.93656 0.00019 0.00000 0.00014 0.00013 1.93669

A82 1.93656 0.00019 0.00000 0.00014 0.00013 1.93669

A83 1.93538 0.00073 0.00000 0.00666 0.00664 1.94202

A84 1.87099 -0.00090 0.00000 -0.00966 -0.00967 1.86132

A85 1.89112 -0.00014 0.00000 0.00112 0.00111 1.89223

A86 1.89112 -0.00014 0.00000 0.00112 0.00111 1.89223

A87 1.93656 0.00036 0.00000 0.00115 0.00114 1.93770

A88 1.93656 0.00036 0.00000 0.00115 0.00114 1.93770

A89 1.93538 0.00063 0.00000 0.00618 0.00617 1.94154

A90 1.87099 -0.00111 0.00000 -0.01119 -0.01119 1.85980

A91 1.89112 -0.00016 0.00000 0.00107 0.00106 1.89217

A92 1.89112 -0.00016 0.00000 0.00107 0.00106 1.89217

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 -0.00046 0.00000 -0.00626 -0.00626 1.03276

D31 -1.03902 0.00046 0.00000 0.00626 0.00626 -1.03276

D32 0.00000 0.00000 0.00000 0.00000 -0.00000 0.00000

D33 -2.10257 -0.00046 0.00000 -0.00626 -0.00626 -2.10884

D34 2.10257 0.00046 0.00000 0.00626 0.00626 2.10884

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

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D54 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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D57 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

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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 -0.00044 0.00000 -0.00596 -0.00597 1.03306

D64 -1.03902 0.00044 0.00000 0.00596 0.00597 -1.03306

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D66 -2.10257 -0.00044 0.00000 -0.00596 -0.00597 -2.10854

D67 2.10257 0.00044 0.00000 0.00596 0.00597 2.10854

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

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D78 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

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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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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 -0.00046 0.00000 -0.00626 -0.00626 1.03276

D126 -1.03902 0.00046 0.00000 0.00626 0.00626 -1.03276

D127 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

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D129 2.10257 0.00046 0.00000 0.00626 0.00626 2.10884

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 0.010417 0.000450 NO

RMS Force 0.002165 0.000300 NO

Maximum Displacement 0.046973 0.001800 NO

RMS Displacement 0.009612 0.001200 NO

Predicted change in Energy=-1.648056D-03

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 13:50:57 2019, MaxMem= 2415919104 cpu: 2.0

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.077661 -2.187088 0.000000

2 7 0 -0.741644 -1.861980 -0.000000

3 6 0 -0.002152 -2.994785 0.000000

4 6 0 -0.929107 -4.154076 0.000000

5 6 0 -2.193009 -3.641281 -0.000000

6 7 0 1.336636 -3.111390 -0.000000

7 6 0 2.183081 -2.063534 0.000000

8 7 0 1.860117 -0.745737 -0.000000

9 6 0 3.007804 0.004646 0.000000

10 6 0 4.164962 -0.913882 -0.000000

11 6 0 3.646091 -2.174363 -0.000000

12 7 0 -3.112958 -1.336187 0.000000

13 6 0 -4.164962 0.913882 0.000000

14 6 0 -3.646091 2.174363 0.000000

15 6 0 -2.183081 2.063534 -0.000000

16 7 0 -1.860117 0.745737 0.000000

17 6 0 -3.007804 -0.004646 -0.000000

18 7 0 -1.336636 3.111390 0.000000

19 7 0 0.741644 1.861980 0.000000

20 6 0 0.002152 2.994785 -0.000000

21 6 0 0.929107 4.154076 -0.000000

22 6 0 2.193009 3.641281 0.000000

23 6 0 2.077661 2.187088 -0.000000

24 7 0 3.112958 1.336187 -0.000000

25 30 0 0.000000 0.000000 -0.000000

26 6 0 -0.486413 -5.574462 -0.000000

27 1 0 -3.126300 -4.186877 0.000000

28 6 0 5.587899 -0.478923 0.000000

29 1 0 4.190037 -3.108381 0.000000

30 6 0 -5.587899 0.478923 0.000000

31 1 0 -4.190037 3.108381 -0.000000

32 6 0 0.486413 5.574462 0.000000

33 1 0 3.126300 4.186877 -0.000000

34 1 0 -1.339724 -6.254507 0.000000

35 1 0 0.130514 -5.793618 0.877681

36 1 0 0.130514 -5.793618 -0.877681

37 1 0 5.809359 0.136172 0.877803

38 1 0 5.809359 0.136172 -0.877803

39 1 0 6.263641 -1.335578 -0.000000

40 1 0 -5.809359 -0.136172 0.877803

41 1 0 -5.809359 -0.136172 -0.877803

42 1 0 -6.263641 1.335578 0.000000

43 1 0 -0.130514 5.793618 0.877681

44 1 0 -0.130514 5.793618 -0.877681

45 1 0 1.339724 6.254507 -0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.375003 0.000000

3 C 2.227130 1.352810 0.000000

4 C 2.277766 2.299749 1.484318 0.000000

5 C 1.458761 2.296165 2.284253 1.363967 0.000000

6 N 3.537197 2.424928 1.343857 2.494150 3.569199

7 C 4.262532 2.931662 2.375389 3.749143 4.651822

8 N 4.193279 2.831106 2.919977 4.404151 4.981165

9 C 5.537657 4.188395 4.249285 5.726625 6.351475

10 C 6.371137 4.997367 4.657789 6.037251 6.918273

11 C 5.723766 4.398841 3.739354 4.985148 6.020543

12 N 1.340102 2.428907 3.525346 3.565067 2.481888

13 C 3.738026 4.407325 5.710224 6.012899 4.963679

14 C 4.634892 4.972713 6.324427 6.887027 5.994428

15 C 4.251929 4.181794 5.508452 6.342801 5.704824

16 N 2.940882 2.837458 4.176546 4.987479 4.399630

17 C 2.372386 2.930046 4.239678 4.640985 3.726795

18 N 5.350046 5.008835 6.250298 7.276886 6.806757

19 N 4.933906 4.008494 4.913390 6.243744 6.236832

20 C 5.583675 4.913390 5.989571 7.209261 6.989714

21 C 7.017906 6.243744 7.209261 8.513421 8.397333

22 C 7.225545 6.236832 6.989714 8.397333 8.501345

23 C 6.033250 4.933906 5.583675 7.017906 7.225545

24 N 6.273435 5.008616 5.334907 6.817718 7.275196

25 Zn 3.016625 2.004247 2.994785 4.256710 4.250672

26 C 3.742509 3.721245 2.624737 1.487776 2.578693

27 H 2.258052 3.330424 3.343857 2.197438 1.081067

28 C 7.853574 6.478886 6.130108 7.481852 8.398990

29 H 6.335047 5.086747 4.193728 5.224855 6.405252

30 C 4.407878 5.382008 6.577782 6.570314 5.338667

31 H 5.701239 6.049455 7.401825 7.960964 7.038897

32 C 8.174114 7.537162 8.583163 9.830979 9.597356

33 H 8.228525 7.179809 7.833484 9.274579 9.464412

34 H 4.133818 4.433057 3.523477 2.140191 2.749008

35 H 4.318960 4.121742 2.936221 2.140378 3.286584

36 H 4.318960 4.121742 2.936221 2.140378 3.286584

37 H 8.268806 6.904983 6.659361 8.036397 8.892557

38 H 8.268806 6.904983 6.659361 8.036397 8.892557

39 H 8.384652 7.025036 6.481754 7.725254 8.765341

40 H 4.347685 5.425005 6.531910 6.382080 5.112173

41 H 4.347685 5.425005 6.531910 6.382080 5.112173

42 H 5.470979 6.380974 7.613034 7.654643 6.429555

43 H 8.261560 7.729941 8.833053 10.018218 9.697501

44 H 8.261560 7.729941 8.833053 10.018218 9.697501

45 H 9.107088 8.379109 9.346124 10.652990 10.507466

6 7 8 9 10

6 N 0.000000

7 C 1.347023 0.000000

8 N 2.422880 1.356796 0.000000

9 C 3.535885 2.226553 1.371226 0.000000

10 C 3.581685 2.291191 2.310970 1.477399 0.000000

11 C 2.492308 1.467202 2.287067 2.270571 1.363099

12 N 4.790641 5.345752 5.008005 6.265905 7.290162

13 C 6.816920 7.011609 6.249473 7.230165 8.528092

14 C 7.264073 7.206873 6.232601 6.998713 8.399393

15 C 6.258455 6.008000 4.923358 5.584291 7.011609

16 N 5.009657 4.923358 4.008072 4.924010 6.249473

17 C 5.340976 5.584291 4.924010 6.015615 7.230165

18 N 6.772694 6.258455 5.009657 5.340976 6.816920

19 N 5.008835 4.181794 2.837458 2.930046 4.407325

20 C 6.250298 5.508452 4.176546 4.239678 5.710224

21 C 7.276886 6.342801 4.987479 4.640985 6.012899

22 C 6.806757 5.704824 4.399630 3.726795 4.963679

23 C 5.350046 4.251929 2.940882 2.372386 3.738026

24 N 4.789182 3.524596 2.429818 1.335686 2.483852

25 Zn 3.386347 3.004000 2.004036 3.007807 4.264046

26 C 3.064349 4.410535 5.368687 6.583009 6.584551

27 H 4.590694 5.718226 6.058531 7.429407 7.992183

28 C 5.000311 3.755500 3.737318 2.625020 1.487931

29 H 2.853402 2.262649 3.318225 3.329957 2.194643

30 C 7.799971 8.176320 7.548029 8.608777 9.851812

31 H 8.320438 8.207639 7.173465 7.838500 9.272789

32 C 8.727366 7.824172 6.467765 6.113940 7.458574

33 H 7.514493 6.321179 5.092533 4.183909 5.205435

34 H 4.128207 5.474889 6.370678 7.620893 7.669671

35 H 3.069104 4.347054 5.407676 6.532151 6.392099

36 H 3.069104 4.347054 5.407676 6.532151 6.392099

37 H 5.596646 4.331182 4.140629 2.938800 2.139437

38 H 5.596646 4.331182 4.140629 2.938800 2.139437

39 H 5.237259 4.144984 4.442852 3.520892 2.140627

40 H 7.790232 8.268274 7.743576 8.861869 10.043030

41 H 7.790232 8.268274 7.743576 8.861869 10.043030

42 H 8.805666 9.105003 8.386139 9.366487 10.668451

43 H 9.067636 8.237590 6.891741 6.643158 8.013238

44 H 9.067636 8.237590 6.891741 6.643158 8.013238

45 H 9.365898 8.360686 7.019560 6.468636 7.705048

11 12 13 14 15

11 C 0.000000

12 N 6.810821 0.000000

13 C 8.399393 2.483852 0.000000

14 C 8.490426 3.550801 1.363099 0.000000

15 C 7.206873 3.524596 2.291191 1.467202 0.000000

16 N 6.232601 2.429818 2.310970 2.287067 1.356796

17 C 6.998713 1.335686 1.477399 2.270571 2.226553

18 N 7.264073 4.789182 3.581685 2.492308 1.347023

19 N 4.972713 5.008616 4.997367 4.398841 2.931662

20 C 6.324427 5.334907 4.657789 3.739354 2.375389

21 C 6.887027 6.817718 6.037251 4.985148 3.749143

22 C 5.994428 7.275196 6.918273 6.020543 4.651822

23 C 4.634892 6.273435 6.371137 5.723766 4.262532

24 N 3.550801 6.775221 7.290162 6.810821 5.345752

25 Zn 4.245213 3.387611 4.264046 4.245213 3.004000

26 C 5.351473 4.986153 7.458574 8.368265 7.824172

27 H 7.065089 2.850721 5.205435 6.382441 6.321179

28 C 2.577815 8.742987 9.851812 9.607627 8.176320

29 H 1.080864 7.514946 9.272789 9.450518 8.207639

30 C 9.607627 3.069195 1.487931 2.577815 3.755500

31 H 9.450518 4.573214 2.194643 1.080864 2.262649

32 C 8.368265 7.791826 6.584551 5.351473 4.410535

33 H 6.382441 8.332621 7.992183 7.065089 5.718226

34 H 6.442510 5.228215 7.705048 8.738717 8.360686

35 H 5.121388 5.582036 8.013238 8.861252 8.237590

36 H 5.121388 5.582036 8.013238 8.861252 8.237590

37 H 3.284636 9.085490 10.043030 9.712378 8.268274

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40 H 9.712378 3.079148 2.139437 3.284636 4.331182

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42 H 10.512967 4.130997 2.140627 2.748660 4.144984

43 H 8.861252 7.778137 6.392099 5.121388 4.347054

44 H 8.861252 7.778137 6.392099 5.121388 4.347054

45 H 8.738717 8.800285 7.669671 6.442510 5.474889

16 17 18 19 20

16 N 0.000000

17 C 1.371226 0.000000

18 N 2.422880 3.535885 0.000000

19 N 2.831106 4.188395 2.424928 0.000000

20 C 2.919977 4.249285 1.343857 1.352810 0.000000

21 C 4.404151 5.726625 2.494150 2.299749 1.484318

22 C 4.981165 6.351475 3.569199 2.296165 2.284253

23 C 4.193279 5.537657 3.537197 1.375003 2.227130

24 N 5.008005 6.265905 4.790641 2.428907 3.525346

25 Zn 2.004036 3.007807 3.386347 2.004247 2.994785

26 C 6.467765 6.113940 8.727366 7.537162 8.583163

27 H 5.092533 4.183909 7.514493 7.179809 7.833484

28 C 7.548029 8.608777 7.799971 5.382008 6.577782

29 H 7.173465 7.838500 8.320438 6.049455 7.401825

30 C 3.737318 2.625020 5.000311 6.478886 6.130108

31 H 3.318225 3.329957 2.853402 5.086747 4.193728

32 C 5.368687 6.583009 3.064349 3.721245 2.624737

33 H 6.058531 7.429407 4.590694 3.330424 3.343857

34 H 7.019560 6.468636 9.365898 8.379109 9.346124

35 H 6.891741 6.643158 9.067636 7.729941 8.833053

36 H 6.891741 6.643158 9.067636 7.729941 8.833053

37 H 7.743576 8.861869 7.790232 5.425005 6.531910

38 H 7.743576 8.861869 7.790232 5.425005 6.531910

39 H 8.386139 9.366487 8.805666 6.380974 7.613034

40 H 4.140629 2.938800 5.596646 6.904983 6.659361

41 H 4.140629 2.938800 5.596646 6.904983 6.659361

42 H 4.442852 3.520892 5.237259 7.025036 6.481754

43 H 5.407676 6.532151 3.069104 4.121742 2.936221

44 H 5.407676 6.532151 3.069104 4.121742 2.936221

45 H 6.370678 7.620893 4.128207 4.433057 3.523477

21 22 23 24 25

21 C 0.000000

22 C 1.363967 0.000000

23 C 2.277766 1.458761 0.000000

24 N 3.565067 2.481888 1.340102 0.000000

25 Zn 4.256710 4.250672 3.016625 3.387611 0.000000

26 C 9.830979 9.597356 8.174114 7.791826 5.595644

27 H 9.274579 9.464412 8.228525 8.332621 5.225293

28 C 6.570314 5.338667 4.407878 3.069195 5.608385

29 H 7.960964 7.038897 5.701239 4.573214 5.217130

30 C 7.481852 8.398990 7.853574 8.742987 5.608385

31 H 5.224855 6.405252 6.335047 7.514946 5.217130

32 C 1.487776 2.578693 3.742509 4.986153 5.595644

33 H 2.197438 1.081067 2.258052 2.850721 5.225293

34 H 10.652990 10.507466 9.107088 8.800285 6.396383

35 H 10.018218 9.697501 8.261560 7.778137 5.861175

36 H 10.018218 9.697501 8.261560 7.778137 5.861175

37 H 6.382080 5.112173 4.347685 3.079148 5.876881

38 H 6.382080 5.112173 4.347685 3.079148 5.876881

39 H 7.654643 6.429555 5.470979 4.130997 6.404449

40 H 8.036397 8.892557 8.268806 9.085490 5.876881

41 H 8.036397 8.892557 8.268806 9.085490 5.876881

42 H 7.725254 8.765341 8.384652 9.376600 6.404449

43 H 2.140378 3.286584 4.318960 5.582036 5.861175

44 H 2.140378 3.286584 4.318960 5.582036 5.861175

45 H 2.140191 2.749008 4.133818 5.228215 6.396383

26 27 28 29 30

26 C 0.000000

27 H 2.982347 0.000000

28 C 7.928542 9.470278 0.000000

29 H 5.286846 7.395400 2.977930 0.000000

30 C 7.916352 5.275335 11.216770 10.415219 0.000000

31 H 9.439735 7.372403 10.415219 10.434260 2.977930

32 C 11.191288 10.408431 7.916352 9.439735 7.928542

33 H 10.408431 10.450586 5.275335 7.372403 9.470278

34 H 1.091147 2.732571 9.019386 6.362104 7.961537

35 H 1.094967 3.736144 7.668074 4.945761 8.533191

36 H 1.094967 3.736144 7.668074 4.945761 8.533191

37 H 8.545094 9.965203 1.094498 3.730934 11.436149

38 H 8.545094 9.965203 1.094498 3.730934 11.436149

39 H 7.970657 9.813302 1.091094 2.728125 11.989638

40 H 7.660241 4.937363 11.436149 10.468643 1.094498

41 H 7.660241 4.937363 11.436149 10.468643 1.094498

42 H 9.006943 6.351411 11.989638 11.359057 1.091094

43 H 11.407464 10.457310 8.533191 9.933935 7.668074

44 H 11.407464 10.457310 8.533191 9.933935 7.668074

45 H 11.969098 11.356402 7.961537 9.787133 9.019386

31 32 33 34 35

31 H 0.000000

32 C 5.286846 0.000000

33 H 7.395400 2.982347 0.000000

34 H 9.787133 11.969098 11.356402 0.000000

35 H 9.933935 11.407464 10.457310 1.773230 0.000000

36 H 9.933935 11.407464 10.457310 1.773230 1.755362

37 H 10.468643 7.660241 4.937363 9.629159 8.210462

38 H 10.468643 7.660241 4.937363 9.629159 8.396036

39 H 11.359057 9.006943 6.351411 9.055773 7.632804

40 H 3.730934 8.545094 9.965203 7.627725 8.202974

41 H 3.730934 8.545094 9.965203 7.627725 8.388713

42 H 2.728125 7.970657 9.813302 9.047340 9.616703

43 H 4.945761 1.094967 3.736144 12.140422 11.590176

44 H 4.945761 1.094967 3.736144 12.140422 11.722349

45 H 6.362104 1.091147 2.732571 12.792767 12.140422

36 37 38 39 40

36 H 0.000000

37 H 8.396036 0.000000

38 H 8.210462 1.755606 0.000000

39 H 7.632804 1.772840 1.772840 0.000000

40 H 8.388713 11.621909 11.753762 12.164146 0.000000

41 H 8.202974 11.753762 11.621909 12.164146 1.755606

42 H 9.616703 12.164146 12.164146 12.808899 1.772840

43 H 11.722349 8.202974 8.388713 9.616703 8.210462

44 H 11.590176 8.388713 8.202974 9.616703 8.396036

45 H 12.140422 7.627725 7.627725 9.047340 9.629159

41 42 43 44 45

41 H 0.000000

42 H 1.772840 0.000000

43 H 8.396036 7.632804 0.000000

44 H 8.210462 7.632804 1.755362 0.000000

45 H 9.629159 9.055773 1.773230 1.773230 0.000000

Stoichiometry C20H16N8Zn(3)

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= 5.36D-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 -2.803157 1.114601 0.000000

2 7 0 -2.004242 -0.004492 0.000000

3 6 0 -2.780517 -1.112414 0.000000

4 6 0 -4.201490 -0.683421 0.000000

5 6 0 -4.195842 0.680535 0.000000

6 7 0 -2.390562 -2.398450 0.000000

7 6 0 -1.102980 -2.794181 0.000000

8 7 0 0.000000 -2.004036 0.000000

9 6 0 1.123569 -2.790071 0.000000

10 6 0 0.701603 -4.205929 0.000000

11 6 0 -0.661438 -4.193368 0.000000

12 7 0 -2.398616 2.392185 0.000000

13 6 0 -0.701603 4.205929 0.000000

14 6 0 0.661438 4.193368 0.000000

15 6 0 1.102980 2.794181 0.000000

16 7 0 0.000000 2.004036 0.000000

17 6 0 -1.123569 2.790071 0.000000

18 7 0 2.390562 2.398450 0.000000

19 7 0 2.004242 0.004492 0.000000

20 6 0 2.780517 1.112414 0.000000

21 6 0 4.201490 0.683421 0.000000

22 6 0 4.195842 -0.680535 0.000000

23 6 0 2.803157 -1.114601 0.000000

24 7 0 2.398616 -2.392185 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -5.355139 -1.622873 0.000000

27 1 0 -5.049550 1.343776 0.000000

28 6 0 1.634825 -5.364823 0.000000

29 1 0 -1.325969 -5.045815 0.000000

30 6 0 -1.634825 5.364823 0.000000

31 1 0 1.325969 5.045815 0.000000

32 6 0 5.355139 1.622873 0.000000

33 1 0 5.049550 -1.343776 0.000000

34 1 0 -6.303879 -1.083899 0.000000

35 1 0 -5.328986 -2.277048 0.877681

36 1 0 -5.328986 -2.277048 -0.877681

37 1 0 2.288157 -5.341491 0.877803

38 1 0 2.288157 -5.341491 -0.877803

39 1 0 1.091146 -6.310814 0.000000

40 1 0 -2.288157 5.341491 0.877803

41 1 0 -2.288157 5.341491 -0.877803

42 1 0 -1.091146 6.310814 0.000000

43 1 0 5.328986 2.277048 0.877681

44 1 0 5.328986 2.277048 -0.877681

45 1 0 6.303879 1.083899 0.000000

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

Rotational constants (GHZ): 0.1830837 0.1819710 0.0914680

Leave Link 202 at Tue Sep 17 13:50:57 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 101 beta electrons

nuclear repulsion energy 2762.5458462227 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= -0.1142430034 Hartrees.

Nuclear repulsion after empirical dispersion term = 2762.4316032193 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 = 3492

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.13D-08

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 130

GePol: Fraction of low-weight points (<1% of avg) = 3.72%

GePol: Cavity surface area = 381.761 Ang\*\*2

GePol: Cavity volume = 378.931 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0107031714 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2762.4209000479 Hartrees.

Leave Link 301 at Tue Sep 17 13:50:57 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= 15327 LenP2D= 41262.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.83D-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 13:50:58 2019, MaxMem= 2415919104 cpu: 12.3

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 13:50:58 2019, MaxMem= 2415919104 cpu: 1.2

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= 0.000000 -0.000000 -0.000000

Rot= 0.981935 -0.000000 0.000000 -0.189219 Ang= -21.81 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 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0409 S= 1.0136

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= -1276.14608698511

Leave Link 401 at Tue Sep 17 13:51:00 2019, MaxMem= 2415919104 cpu: 41.9

(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= 36582192.

Iteration 1 A\*A^-1 deviation from unit magnitude is 1.04D-14 for 3491.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.69D-15 for 1404 1384.

Iteration 1 A^-1\*A deviation from unit magnitude is 1.04D-14 for 3491.

Iteration 1 A^-1\*A deviation from orthogonality is 7.79D-14 for 3272 3133.

E= -1275.83896386623

DIIS: error= 8.57D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.83896386623 IErMin= 1 ErrMin= 8.57D-04

ErrMax= 8.57D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.85D-03 BMatP= 2.85D-03

IDIUse=3 WtCom= 9.91D-01 WtEn= 8.57D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.297 Goal= None Shift= 0.000

Gap= 0.396 Goal= None Shift= 0.000

RMSDP=8.88D-05 MaxDP=2.54D-03 OVMax= 2.32D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 8.88D-05 CP: 1.00D+00

E= -1275.83992382435 Delta-E= -0.000959958123 Rises=F Damp=F

DIIS: error= 5.10D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.83992382435 IErMin= 2 ErrMin= 5.10D-04

ErrMax= 5.10D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.75D-04 BMatP= 2.85D-03

IDIUse=3 WtCom= 9.95D-01 WtEn= 5.10D-03

Coeff-Com: 0.144D+00 0.856D+00

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

Coeff: 0.143D+00 0.857D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=2.71D-05 MaxDP=1.22D-03 DE=-9.60D-04 OVMax= 5.74D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.70D-05 CP: 1.00D+00 9.90D-01

E= -1275.83991780958 Delta-E= 0.000006014775 Rises=F Damp=F

DIIS: error= 7.94D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1275.83992382435 IErMin= 2 ErrMin= 5.10D-04

ErrMax= 7.94D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.70D-04 BMatP= 3.75D-04

IDIUse=3 WtCom= 2.62D-01 WtEn= 7.38D-01

Coeff-Com: -0.111D-01 0.533D+00 0.478D+00

Coeff-En: 0.000D+00 0.515D+00 0.485D+00

Coeff: -0.290D-02 0.519D+00 0.483D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.97D-05 MaxDP=8.96D-04 DE= 6.01D-06 OVMax= 5.07D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.28D-05 CP: 1.00D+00 1.05D+00 4.82D-01

E= -1275.84002356061 Delta-E= -0.000105751034 Rises=F Damp=F

DIIS: error= 2.74D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84002356061 IErMin= 4 ErrMin= 2.74D-04

ErrMax= 2.74D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.62D-05 BMatP= 3.75D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 2.74D-03

Coeff-Com: -0.133D-01 0.214D+00 0.281D+00 0.518D+00

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

Coeff: -0.133D-01 0.213D+00 0.281D+00 0.520D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=6.58D-06 MaxDP=2.14D-04 DE=-1.06D-04 OVMax= 2.06D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 5.04D-06 CP: 1.00D+00 1.05D+00 6.18D-01 8.35D-01

E= -1275.84003448846 Delta-E= -0.000010927845 Rises=F Damp=F

DIIS: error= 8.59D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84003448846 IErMin= 5 ErrMin= 8.59D-05

ErrMax= 8.59D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.19D-06 BMatP= 3.62D-05

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

Coeff-Com: -0.362D-02 0.435D-02 0.594D-01 0.267D+00 0.673D+00

Coeff: -0.362D-02 0.435D-02 0.594D-01 0.267D+00 0.673D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=3.47D-06 MaxDP=1.63D-04 DE=-1.09D-05 OVMax= 2.12D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.14D-06 CP: 1.00D+00 1.06D+00 6.41D-01 1.02D+00 1.15D+00

E= -1275.84003771759 Delta-E= -0.000003229132 Rises=F Damp=F

DIIS: error= 6.04D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84003771759 IErMin= 6 ErrMin= 6.04D-05

ErrMax= 6.04D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.11D-07 BMatP= 4.19D-06

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

Coeff-Com: 0.251D-02-0.481D-01-0.442D-01-0.683D-01 0.109D+00 0.105D+01

Coeff: 0.251D-02-0.481D-01-0.442D-01-0.683D-01 0.109D+00 0.105D+01

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=3.67D-06 MaxDP=1.89D-04 DE=-3.23D-06 OVMax= 2.31D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.33D-06 CP: 1.00D+00 1.07D+00 6.87D-01 1.17D+00 1.59D+00

CP: 1.61D+00

E= -1275.84003955401 Delta-E= -0.000001836418 Rises=F Damp=F

DIIS: error= 3.07D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84003955401 IErMin= 7 ErrMin= 3.07D-05

ErrMax= 3.07D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.18D-07 BMatP= 8.11D-07

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

Coeff-Com: 0.352D-02-0.409D-01-0.607D-01-0.168D+00-0.219D+00 0.747D+00

Coeff-Com: 0.738D+00

Coeff: 0.352D-02-0.409D-01-0.607D-01-0.168D+00-0.219D+00 0.747D+00

Coeff: 0.738D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=3.02D-06 MaxDP=1.42D-04 DE=-1.84D-06 OVMax= 1.63D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 8.43D-07 CP: 1.00D+00 1.07D+00 7.16D-01 1.28D+00 1.89D+00

CP: 2.37D+00 1.54D+00

E= -1275.84004041532 Delta-E= -0.000000861319 Rises=F Damp=F

DIIS: error= 1.65D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84004041532 IErMin= 8 ErrMin= 1.65D-05

ErrMax= 1.65D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.46D-07 BMatP= 6.18D-07

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

Coeff-Com: 0.519D-03 0.344D-02-0.654D-02-0.409D-01-0.134D+00-0.485D-01

Coeff-Com: 0.362D+00 0.863D+00

Coeff: 0.519D-03 0.344D-02-0.654D-02-0.409D-01-0.134D+00-0.485D-01

Coeff: 0.362D+00 0.863D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.89D-06 MaxDP=7.29D-05 DE=-8.61D-07 OVMax= 1.29D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 5.47D-07 CP: 1.00D+00 1.07D+00 7.28D-01 1.33D+00 2.05D+00

CP: 2.81D+00 2.27D+00 1.51D+00

E= -1275.84004065964 Delta-E= -0.000000244310 Rises=F Damp=F

DIIS: error= 1.37D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84004065964 IErMin= 9 ErrMin= 1.37D-05

ErrMax= 1.37D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.69D-08 BMatP= 1.46D-07

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

Coeff-Com: -0.899D-03 0.164D-01 0.173D-01 0.340D-01 0.327D-02-0.278D+00

Coeff-Com: -0.180D-01 0.510D+00 0.717D+00

Coeff: -0.899D-03 0.164D-01 0.173D-01 0.340D-01 0.327D-02-0.278D+00

Coeff: -0.180D-01 0.510D+00 0.717D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.18D-06 MaxDP=4.40D-05 DE=-2.44D-07 OVMax= 9.07D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 3.56D-07 CP: 1.00D+00 1.07D+00 7.33D-01 1.35D+00 2.14D+00

CP: 3.00D+00 2.72D+00 2.10D+00 1.63D+00

E= -1275.84004075214 Delta-E= -0.000000092510 Rises=F Damp=F

DIIS: error= 1.10D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84004075214 IErMin=10 ErrMin= 1.10D-05

ErrMax= 1.10D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.18D-08 BMatP= 5.69D-08

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

Coeff-Com: -0.302D-03 0.293D-02 0.524D-02 0.158D-01 0.327D-01-0.596D-01

Coeff-Com: -0.861D-01-0.790D-01 0.184D+00 0.984D+00

Coeff: -0.302D-03 0.293D-02 0.524D-02 0.158D-01 0.327D-01-0.596D-01

Coeff: -0.861D-01-0.790D-01 0.184D+00 0.984D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.08D-06 MaxDP=4.08D-05 DE=-9.25D-08 OVMax= 8.69D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 3.94D-07 CP: 1.00D+00 1.07D+00 7.37D-01 1.36D+00 2.20D+00

CP: 3.00D+00 3.00D+00 2.65D+00 2.46D+00 2.19D+00

E= -1275.84004080873 Delta-E= -0.000000056590 Rises=F Damp=F

DIIS: error= 8.92D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84004080873 IErMin=11 ErrMin= 8.92D-06

ErrMax= 8.92D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.57D-09 BMatP= 1.18D-08

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

Coeff-Com: 0.759D-04-0.280D-02-0.184D-02-0.177D-03 0.148D-01 0.470D-01

Coeff-Com: -0.356D-01-0.157D+00-0.106D+00 0.361D+00 0.880D+00

Coeff: 0.759D-04-0.280D-02-0.184D-02-0.177D-03 0.148D-01 0.470D-01

Coeff: -0.356D-01-0.157D+00-0.106D+00 0.361D+00 0.880D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=8.30D-07 MaxDP=3.14D-05 DE=-5.66D-08 OVMax= 6.73D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 2.91D-07 CP: 1.00D+00 1.07D+00 7.40D-01 1.37D+00 2.24D+00

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

CP: 1.99D+00

E= -1275.84004084338 Delta-E= -0.000000034643 Rises=F Damp=F

DIIS: error= 7.39D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84004084338 IErMin=12 ErrMin= 7.39D-06

ErrMax= 7.39D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.94D-09 BMatP= 6.57D-09

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

Coeff-Com: 0.270D-03-0.396D-02-0.521D-02-0.116D-01-0.180D-01 0.717D-01

Coeff-Com: 0.373D-01-0.246D-01-0.187D+00-0.560D+00 0.585D+00 0.112D+01

Coeff: 0.270D-03-0.396D-02-0.521D-02-0.116D-01-0.180D-01 0.717D-01

Coeff: 0.373D-01-0.246D-01-0.187D+00-0.560D+00 0.585D+00 0.112D+01

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.25D-06 MaxDP=4.78D-05 DE=-3.46D-08 OVMax= 1.02D-03

Cycle 13 Pass 1 IDiag 1:

RMSU= 7.49D-07 CP: 1.00D+00 1.07D+00 7.44D-01 1.38D+00 2.30D+00

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

CP: 3.00D+00 3.00D+00

E= -1275.84004088355 Delta-E= -0.000000040171 Rises=F Damp=F

DIIS: error= 5.04D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84004088355 IErMin=13 ErrMin= 5.04D-06

ErrMax= 5.04D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.38D-09 BMatP= 4.94D-09

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

Coeff-Com: 0.965D-04 0.505D-03-0.126D-02-0.619D-02-0.280D-01-0.250D-02

Coeff-Com: 0.557D-01 0.150D+00 0.335D-02-0.790D+00-0.428D+00 0.678D+00

Coeff-Com: 0.137D+01

Coeff: 0.965D-04 0.505D-03-0.126D-02-0.619D-02-0.280D-01-0.250D-02

Coeff: 0.557D-01 0.150D+00 0.335D-02-0.790D+00-0.428D+00 0.678D+00

Coeff: 0.137D+01

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.78D-06 MaxDP=6.76D-05 DE=-4.02D-08 OVMax= 1.45D-03

Cycle 14 Pass 1 IDiag 1:

RMSU= 9.60D-07 CP: 1.00D+00 1.07D+00 7.50D-01 1.40D+00 2.39D+00

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

CP: 3.00D+00 3.00D+00 2.86D+00

E= -1275.84004091502 Delta-E= -0.000000031472 Rises=F Damp=F

DIIS: error= 1.86D-06 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84004091502 IErMin=14 ErrMin= 1.86D-06

ErrMax= 1.86D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.04D-10 BMatP= 2.38D-09

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

Coeff-Com: -0.443D-04 0.169D-02 0.134D-02 0.130D-02-0.691D-02-0.249D-01

Coeff-Com: 0.138D-01 0.789D-01 0.686D-01-0.222D+00-0.404D+00-0.180D-01

Coeff-Com: 0.692D+00 0.818D+00

Coeff: -0.443D-04 0.169D-02 0.134D-02 0.130D-02-0.691D-02-0.249D-01

Coeff: 0.138D-01 0.789D-01 0.686D-01-0.222D+00-0.404D+00-0.180D-01

Coeff: 0.692D+00 0.818D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=6.88D-07 MaxDP=2.64D-05 DE=-3.15D-08 OVMax= 5.59D-04

Cycle 15 Pass 1 IDiag 1:

RMSU= 4.40D-07 CP: 1.00D+00 1.07D+00 7.52D-01 1.41D+00 2.42D+00

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

CP: 3.00D+00 3.00D+00 3.00D+00 1.39D+00

E= -1275.84004091918 Delta-E= -0.000000004159 Rises=F Damp=F

DIIS: error= 5.19D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.84004091918 IErMin=15 ErrMin= 5.19D-07

ErrMax= 5.19D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.62D-10 BMatP= 6.04D-10

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

Coeff-Com: -0.392D-04 0.777D-03 0.888D-03 0.164D-02 0.120D-02-0.131D-01

Coeff-Com: -0.178D-02 0.138D-01 0.385D-01 0.311D-01-0.153D+00-0.133D+00

Coeff-Com: 0.959D-01 0.429D+00 0.688D+00

Coeff: -0.392D-04 0.777D-03 0.888D-03 0.164D-02 0.120D-02-0.131D-01

Coeff: -0.178D-02 0.138D-01 0.385D-01 0.311D-01-0.153D+00-0.133D+00

Coeff: 0.959D-01 0.429D+00 0.688D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=2.33D-07 MaxDP=8.93D-06 DE=-4.16D-09 OVMax= 1.89D-04

Cycle 16 Pass 1 IDiag 1:

RMSU= 1.64D-08 CP: 1.00D+00 1.07D+00 7.53D-01 1.41D+00 2.44D+00

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

CP: 3.00D+00 3.00D+00 3.00D+00 1.52D+00 1.41D+00

E= -1275.84004091960 Delta-E= -0.000000000420 Rises=F Damp=F

DIIS: error= 1.42D-07 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1275.84004091960 IErMin=16 ErrMin= 1.42D-07

ErrMax= 1.42D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.52D-11 BMatP= 1.62D-10

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

Coeff-Com: -0.108D-04 0.212D-05 0.157D-03 0.656D-03 0.258D-02-0.296D-03

Coeff-Com: -0.400D-02-0.140D-01 0.236D-02 0.729D-01 0.153D-01-0.511D-01

Coeff-Com: -0.117D+00 0.230D-01 0.351D+00 0.719D+00

Coeff: -0.108D-04 0.212D-05 0.157D-03 0.656D-03 0.258D-02-0.296D-03

Coeff: -0.400D-02-0.140D-01 0.236D-02 0.729D-01 0.153D-01-0.511D-01

Coeff: -0.117D+00 0.230D-01 0.351D+00 0.719D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=2.43D-08 MaxDP=9.01D-07 DE=-4.20D-10 OVMax= 1.82D-05

Cycle 17 Pass 1 IDiag 1:

RMSU= 7.47D-09 CP: 1.00D+00 1.07D+00 7.53D-01 1.41D+00 2.44D+00

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

CP: 3.00D+00 3.00D+00 3.00D+00 1.53D+00 1.46D+00

CP: 9.34D-01

E= -1275.84004091962 Delta-E= -0.000000000022 Rises=F Damp=F

DIIS: error= 8.82D-08 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=17 EnMin= -1275.84004091962 IErMin=17 ErrMin= 8.82D-08

ErrMax= 8.82D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.89D-12 BMatP= 3.52D-11

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

Coeff-Com: 0.149D-05-0.151D-03-0.105D-03 0.133D-04 0.107D-02 0.229D-02

Coeff-Com: -0.138D-02-0.101D-01-0.649D-02 0.341D-01 0.328D-01-0.493D-03

Coeff-Com: -0.818D-01-0.678D-01 0.563D-01 0.397D+00 0.645D+00

Coeff: 0.149D-05-0.151D-03-0.105D-03 0.133D-04 0.107D-02 0.229D-02

Coeff: -0.138D-02-0.101D-01-0.649D-02 0.341D-01 0.328D-01-0.493D-03

Coeff: -0.818D-01-0.678D-01 0.563D-01 0.397D+00 0.645D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.72D-08 MaxDP=6.67D-07 DE=-2.18D-11 OVMax= 1.37D-05

Cycle 18 Pass 1 IDiag 1:

RMSU= 3.06D-09 CP: 1.00D+00 1.07D+00 7.53D-01 1.41D+00 2.44D+00

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

CP: 3.00D+00 3.00D+00 3.00D+00 1.54D+00 1.49D+00

CP: 1.02D+00 1.22D+00

E= -1275.84004091962 Delta-E= 0.000000000000 Rises=F Damp=F

DIIS: error= 5.14D-08 at cycle 18 NSaved= 18.

NSaved=18 IEnMin=17 EnMin= -1275.84004091962 IErMin=18 ErrMin= 5.14D-08

ErrMax= 5.14D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.63D-12 BMatP= 8.89D-12

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

Coeff-Com: 0.425D-05-0.573D-04-0.982D-04-0.193D-03-0.414D-03 0.808D-03

Coeff-Com: 0.897D-03 0.721D-03-0.346D-02-0.871D-02 0.585D-02 0.166D-01

Coeff-Com: 0.469D-02-0.309D-01-0.100D+00-0.831D-01 0.222D+00 0.975D+00

Coeff: 0.425D-05-0.573D-04-0.982D-04-0.193D-03-0.414D-03 0.808D-03

Coeff: 0.897D-03 0.721D-03-0.346D-02-0.871D-02 0.585D-02 0.166D-01

Coeff: 0.469D-02-0.309D-01-0.100D+00-0.831D-01 0.222D+00 0.975D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.08D-08 MaxDP=4.00D-07 DE= 4.55D-13 OVMax= 8.42D-06

Cycle 19 Pass 1 IDiag 1:

RMSU= 1.83D-09 CP: 1.00D+00 1.07D+00 7.53D-01 1.41D+00 2.44D+00

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

CP: 3.00D+00 3.00D+00 3.00D+00 1.55D+00 1.51D+00

CP: 1.07D+00 1.51D+00 1.33D+00

E= -1275.84004091961 Delta-E= 0.000000000006 Rises=F Damp=F

DIIS: error= 2.87D-08 at cycle 19 NSaved= 19.

NSaved=19 IEnMin=17 EnMin= -1275.84004091962 IErMin=19 ErrMin= 2.87D-08

ErrMax= 2.87D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.82D-13 BMatP= 1.63D-12

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

Coeff-Com: 0.188D-05-0.184D-05-0.303D-04-0.908D-04-0.374D-03 0.141D-04

Coeff-Com: 0.641D-03 0.205D-02-0.807D-03-0.982D-02-0.143D-02 0.903D-02

Coeff-Com: 0.148D-01-0.435D-02-0.659D-01-0.105D+00 0.582D-02 0.506D+00

Coeff-Com: 0.649D+00

Coeff: 0.188D-05-0.184D-05-0.303D-04-0.908D-04-0.374D-03 0.141D-04

Coeff: 0.641D-03 0.205D-02-0.807D-03-0.982D-02-0.143D-02 0.903D-02

Coeff: 0.148D-01-0.435D-02-0.659D-01-0.105D+00 0.582D-02 0.506D+00

Coeff: 0.649D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.52D-09 MaxDP=1.05D-07 DE= 6.37D-12 OVMax= 6.33D-07

Error on total polarization charges = 0.06464

SCF Done: E(UB3LYP) = -1275.84004092 A.U. after 19 cycles

NFock= 19 Conv=0.15D-08 -V/T= 1.9659

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0420 S= 1.0139

<L.S>= 0.000000000000E+00

KE= 1.320824175306D+03 PE=-8.576810354531D+03 EE= 3.217725238257D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.72

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0420, after 2.0010

Leave Link 502 at Tue Sep 17 13:52:44 2019, MaxMem= 2415919104 cpu: 1835.0

(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= 15327 LenP2D= 41262.

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 = 247

Leave Link 701 at Tue Sep 17 13:52:48 2019, MaxMem= 2415919104 cpu: 77.1

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 13:52:48 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 13:53:00 2019, MaxMem= 2415919104 cpu: 206.9

(Enter /home/blab/g09/l716.exe)

Dipole = 2.11386464D-13 1.50990331D-14-2.22044605D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.006777958 -0.003171901 -0.000000000

2 7 0.007622212 -0.004063884 -0.000000000

3 6 -0.004185401 0.008172058 -0.000000000

4 6 -0.002284346 -0.003606259 -0.000000000

5 6 0.002194514 0.001758125 -0.000000000

6 7 0.002589093 -0.003623844 -0.000000000

7 6 -0.002886657 0.006683272 0.000000000

8 7 -0.001916836 -0.006952232 -0.000000000

9 6 0.004186756 0.005355923 0.000000000

10 6 -0.000836249 -0.002834288 -0.000000000

11 6 0.003146072 0.000758663 0.000000000

12 7 0.002174006 0.003060219 0.000000000

13 6 0.000836249 0.002834288 0.000000000

14 6 -0.003146072 -0.000758663 0.000000000

15 6 0.002886657 -0.006683272 -0.000000000

16 7 0.001916836 0.006952232 0.000000000

17 6 -0.004186756 -0.005355923 -0.000000000

18 7 -0.002589093 0.003623844 0.000000000

19 7 -0.007622212 0.004063884 -0.000000000

20 6 0.004185401 -0.008172058 0.000000000

21 6 0.002284346 0.003606259 0.000000000

22 6 -0.002194514 -0.001758125 -0.000000000

23 6 0.006777958 0.003171901 -0.000000000

24 7 -0.002174006 -0.003060219 0.000000000

25 30 -0.000000000 -0.000000000 0.000000000

26 6 -0.000117830 0.000785808 0.000000000

27 1 -0.000065216 0.000123383 0.000000000

28 6 -0.000433589 -0.000012179 0.000000000

29 1 -0.000118764 -0.000368852 -0.000000000

30 6 0.000433589 0.000012179 0.000000000

31 1 0.000118764 0.000368852 0.000000000

32 6 0.000117830 -0.000785808 0.000000000

33 1 0.000065216 -0.000123383 -0.000000000

34 1 0.000048776 -0.000138690 -0.000000000

35 1 0.000270551 -0.000096185 -0.000026347

36 1 0.000270551 -0.000096185 0.000026347

37 1 0.000094686 0.000159887 -0.000029730

38 1 0.000094686 0.000159887 0.000029730

39 1 -0.000010553 0.000023648 -0.000000000

40 1 -0.000094686 -0.000159887 -0.000029730

41 1 -0.000094686 -0.000159887 0.000029730

42 1 0.000010553 -0.000023648 0.000000000

43 1 -0.000270551 0.000096185 -0.000026347

44 1 -0.000270551 0.000096185 0.000026347

45 1 -0.000048776 0.000138690 -0.000000000

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

Cartesian Forces: Max 0.008172058 RMS 0.002572355

Leave Link 716 at Tue Sep 17 13:53:00 2019, MaxMem= 2415919104 cpu: 0.4

(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 0.004898626 RMS 0.000933620

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= -2.28D-04 DEPred=-1.65D-03 R= 1.38D-01

Trust test= 1.38D-01 RLast= 9.88D-02 DXMaxT set to 3.00D-01

ITU= 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01336

Eigenvalues --- 0.01337 0.01341 0.01342 0.01605 0.01623

Eigenvalues --- 0.01635 0.01637 0.01774 0.01790 0.01813

Eigenvalues --- 0.01814 0.01890 0.01906 0.01943 0.01945

Eigenvalues --- 0.01998 0.01999 0.02044 0.02047 0.02070

Eigenvalues --- 0.02087 0.02102 0.02112 0.02112 0.02205

Eigenvalues --- 0.02313 0.02316 0.02351 0.02373 0.07218

Eigenvalues --- 0.07218 0.07221 0.07221 0.07273 0.07345

Eigenvalues --- 0.07353 0.07357 0.14498 0.14501 0.15730

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 0.16020

Eigenvalues --- 0.16506 0.18396 0.19447 0.22072 0.22082

Eigenvalues --- 0.23848 0.23851 0.23877 0.24153 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 --- 0.27590 0.31767 0.33191 0.33198 0.33241

Eigenvalues --- 0.33282 0.33282 0.33282 0.33336 0.33724

Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.34337 0.34435 0.34437 0.34437

Eigenvalues --- 0.34526 0.35326 0.35535 0.35549 0.35563

Eigenvalues --- 0.35680 0.35682 0.35682 0.36883 0.38979

Eigenvalues --- 0.39478 0.41711 0.41721 0.44682 0.47931

Eigenvalues --- 0.48951 0.48991 0.49905 0.50416 0.51357

Eigenvalues --- 0.51362 0.51831 0.54017 0.54020 0.54457

Eigenvalues --- 0.56318 0.56333 0.56393 0.56471

DIIS coeff's: 1.42711 -0.42711

Cosine: 1.000 > 0.970

Length: 1.000

GDIIS step was calculated using 2 of the last 2 vectors.

Iteration 1 RMS(Cart)= 0.00451665 RMS(Int)= 0.00001794

Iteration 2 RMS(Cart)= 0.00003217 RMS(Int)= 0.00000817

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000817

ITry= 1 IFail=0 DXMaxC= 2.16D-02 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 5.06D-11 for atom 38.

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

(Linear) (Quad) (Total)

R1 2.59838 0.00452 0.00903 0.00758 0.01660 2.61498

R2 2.75666 -0.00127 -0.00268 -0.00268 -0.00536 2.75130

R3 2.53243 0.00002 -0.00257 0.00188 -0.00068 2.53175

R4 2.55644 -0.00490 -0.00750 -0.00936 -0.01686 2.53958

R5 3.78748 0.00062 -0.00262 0.00611 0.00345 3.79093

R6 2.80495 0.00255 0.00549 0.00665 0.01214 2.81710

R7 2.53952 0.00257 0.00275 0.00520 0.00798 2.54750

R8 2.57752 -0.00045 -0.00429 0.00131 -0.00297 2.57455

R9 2.81149 -0.00030 -0.00303 0.00046 -0.00257 2.80892

R10 2.04292 -0.00001 -0.00124 0.00069 -0.00056 2.04237

R11 2.54550 0.00139 0.00302 0.00216 0.00520 2.55071

R12 2.56397 -0.00385 -0.00566 -0.00758 -0.01324 2.55073

R13 2.77261 0.00224 0.00413 0.00578 0.00991 2.78252

R14 2.59124 0.00358 0.00736 0.00562 0.01298 2.60422

R15 3.78708 0.00055 -0.00279 0.00485 0.00203 3.78911

R16 2.79188 0.00055 -0.00010 0.00301 0.00292 2.79480

R17 2.52408 -0.00193 -0.00384 -0.00239 -0.00622 2.51787

R18 2.57588 -0.00155 -0.00499 -0.00136 -0.00634 2.56954

R19 2.81178 -0.00015 -0.00291 0.00102 -0.00188 2.80990

R20 2.04254 0.00026 -0.00140 0.00184 0.00043 2.04297

R21 2.52408 -0.00193 -0.00384 -0.00239 -0.00622 2.51787

R22 2.57588 -0.00155 -0.00499 -0.00136 -0.00634 2.56954

R23 2.79188 0.00055 -0.00010 0.00301 0.00292 2.79480

R24 2.81178 -0.00015 -0.00291 0.00102 -0.00188 2.80990

R25 2.77261 0.00224 0.00413 0.00578 0.00991 2.78252

R26 2.04254 0.00026 -0.00140 0.00184 0.00043 2.04297

R27 2.56397 -0.00385 -0.00566 -0.00758 -0.01324 2.55073

R28 2.54550 0.00139 0.00302 0.00216 0.00520 2.55071

R29 2.59124 0.00358 0.00736 0.00562 0.01298 2.60422

R30 3.78708 0.00055 -0.00279 0.00485 0.00203 3.78911

R31 2.53952 0.00257 0.00275 0.00520 0.00798 2.54750

R32 2.55644 -0.00490 -0.00750 -0.00936 -0.01686 2.53958

R33 2.59838 0.00452 0.00903 0.00758 0.01660 2.61498

R34 3.78748 0.00062 -0.00262 0.00611 0.00345 3.79093

R35 2.80495 0.00255 0.00549 0.00665 0.01214 2.81710

R36 2.57752 -0.00045 -0.00429 0.00131 -0.00297 2.57455

R37 2.81149 -0.00030 -0.00303 0.00046 -0.00257 2.80892

R38 2.75666 -0.00127 -0.00268 -0.00268 -0.00536 2.75130

R39 2.04292 -0.00001 -0.00124 0.00069 -0.00056 2.04237

R40 2.53243 0.00002 -0.00257 0.00188 -0.00068 2.53175

R41 2.06197 0.00005 -0.00172 0.00118 -0.00053 2.06143

R42 2.06919 0.00015 -0.00375 0.00278 -0.00098 2.06821

R43 2.06919 0.00015 -0.00375 0.00278 -0.00098 2.06821

R44 2.06830 0.00008 -0.00413 0.00272 -0.00142 2.06688

R45 2.06830 0.00008 -0.00413 0.00272 -0.00142 2.06688

R46 2.06187 -0.00002 -0.00176 0.00090 -0.00086 2.06101

R47 2.06830 0.00008 -0.00413 0.00272 -0.00142 2.06688

R48 2.06830 0.00008 -0.00413 0.00272 -0.00142 2.06688

R49 2.06187 -0.00002 -0.00176 0.00090 -0.00086 2.06101

R50 2.06919 0.00015 -0.00375 0.00278 -0.00098 2.06821

R51 2.06919 0.00015 -0.00375 0.00278 -0.00098 2.06821

R52 2.06197 0.00005 -0.00172 0.00118 -0.00053 2.06143

A1 1.88865 -0.00082 -0.00116 -0.00327 -0.00443 1.88422

A2 2.21494 -0.00083 0.00110 -0.00552 -0.00442 2.21052

A3 2.17959 0.00166 0.00006 0.00878 0.00885 2.18844

A4 1.91043 0.00013 0.00173 0.00038 0.00212 1.91256

A5 2.18855 -0.00064 -0.00076 -0.00277 -0.00353 2.18501

A6 2.18421 0.00051 -0.00097 0.00240 0.00141 2.18562

A7 1.88876 0.00070 -0.00329 0.00407 0.00077 1.88953

A8 2.23601 0.00073 0.00708 0.00076 0.00785 2.24387

A9 2.15841 -0.00143 -0.00379 -0.00484 -0.00862 2.14979

A10 1.85986 -0.00055 0.00375 -0.00626 -0.00250 1.85735

A11 2.16497 -0.00068 -0.00546 -0.00031 -0.00577 2.15921

A12 2.25836 0.00124 0.00171 0.00656 0.00827 2.26663

A13 1.87707 0.00055 -0.00103 0.00507 0.00405 1.88112

A14 2.17897 -0.00042 0.00029 -0.00369 -0.00340 2.17557

A15 2.22715 -0.00013 0.00074 -0.00138 -0.00065 2.22650

A16 2.16339 -0.00162 -0.01008 -0.00287 -0.01291 2.15048

A17 2.22178 0.00048 0.00402 0.00113 0.00516 2.22694

A18 2.17466 -0.00127 -0.00205 -0.00507 -0.00711 2.16755

A19 1.88675 0.00079 -0.00198 0.00394 0.00195 1.88870

A20 1.90951 -0.00007 0.00134 -0.00008 0.00128 1.91079

A21 2.19243 0.00057 0.00090 0.00231 0.00320 2.19563

A22 2.18125 -0.00050 -0.00224 -0.00223 -0.00447 2.17677

A23 1.89160 -0.00088 -0.00208 -0.00273 -0.00482 1.88678

A24 2.22866 -0.00016 0.00394 -0.00405 -0.00011 2.22855

A25 2.16292 0.00103 -0.00186 0.00679 0.00494 2.16786

A26 1.85123 0.00039 0.00007 0.00295 0.00302 1.85425

A27 2.17400 -0.00070 -0.00161 -0.00347 -0.00508 2.16892

A28 2.25796 0.00031 0.00154 0.00052 0.00206 2.26002

A29 1.88569 -0.00024 0.00265 -0.00408 -0.00142 1.88427

A30 2.17376 -0.00018 -0.00193 -0.00025 -0.00218 2.17158

A31 2.22373 0.00042 -0.00072 0.00433 0.00360 2.22734

A32 2.17993 0.00146 -0.00301 0.01085 0.00784 2.18777

A33 1.85123 0.00039 0.00007 0.00295 0.00302 1.85425

A34 2.25796 0.00031 0.00154 0.00052 0.00206 2.26002

A35 2.17400 -0.00070 -0.00161 -0.00347 -0.00508 2.16892

A36 1.88569 -0.00024 0.00265 -0.00408 -0.00142 1.88427

A37 2.22373 0.00042 -0.00072 0.00433 0.00360 2.22734

A38 2.17376 -0.00018 -0.00193 -0.00025 -0.00218 2.17158

A39 1.88675 0.00079 -0.00198 0.00394 0.00195 1.88870

A40 2.17466 -0.00127 -0.00205 -0.00507 -0.00711 2.16755

A41 2.22178 0.00048 0.00402 0.00113 0.00516 2.22694

A42 1.90951 -0.00007 0.00134 -0.00008 0.00128 1.91079

A43 2.19243 0.00057 0.00090 0.00231 0.00320 2.19563

A44 2.18125 -0.00050 -0.00224 -0.00223 -0.00447 2.17677

A45 2.16292 0.00103 -0.00186 0.00679 0.00494 2.16786

A46 2.22866 -0.00016 0.00394 -0.00405 -0.00011 2.22855

A47 1.89160 -0.00088 -0.00208 -0.00273 -0.00482 1.88678

A48 2.16339 -0.00162 -0.01008 -0.00287 -0.01291 2.15048

A49 1.91043 0.00013 0.00173 0.00038 0.00212 1.91256

A50 2.18421 0.00051 -0.00097 0.00240 0.00141 2.18562

A51 2.18855 -0.00064 -0.00076 -0.00277 -0.00353 2.18501

A52 2.23601 0.00073 0.00708 0.00076 0.00785 2.24387

A53 2.15841 -0.00143 -0.00379 -0.00484 -0.00862 2.14979

A54 1.88876 0.00070 -0.00329 0.00407 0.00077 1.88953

A55 1.85986 -0.00055 0.00375 -0.00626 -0.00250 1.85735

A56 2.16497 -0.00068 -0.00546 -0.00031 -0.00577 2.15921

A57 2.25836 0.00124 0.00171 0.00656 0.00827 2.26663

A58 1.87707 0.00055 -0.00103 0.00507 0.00405 1.88112

A59 2.22715 -0.00013 0.00074 -0.00138 -0.00065 2.22650

A60 2.17897 -0.00042 0.00029 -0.00369 -0.00340 2.17557

A61 1.88865 -0.00082 -0.00116 -0.00327 -0.00443 1.88422

A62 2.21494 -0.00083 0.00110 -0.00552 -0.00442 2.21052

A63 2.17959 0.00166 0.00006 0.00878 0.00885 2.18844

A64 2.17993 0.00146 -0.00301 0.01085 0.00784 2.18777

A65 1.56856 -0.00066 -0.00096 -0.00373 -0.00471 1.56385

A66 1.57304 0.00066 0.00096 0.00373 0.00471 1.57775

A67 1.57304 0.00066 0.00096 0.00373 0.00471 1.57775

A68 1.56856 -0.00066 -0.00096 -0.00373 -0.00471 1.56385

A69 1.94154 0.00021 0.00263 0.00122 0.00383 1.94538

A70 1.93770 0.00008 0.00049 0.00007 0.00055 1.93825

A71 1.93770 0.00008 0.00049 0.00007 0.00055 1.93825

A72 1.89217 -0.00007 0.00045 -0.00008 0.00036 1.89253

A73 1.89217 -0.00007 0.00045 -0.00008 0.00036 1.89253

A74 1.85980 -0.00028 -0.00478 -0.00130 -0.00608 1.85372

A75 1.93669 0.00012 0.00005 0.00089 0.00094 1.93763

A76 1.93669 0.00012 0.00005 0.00089 0.00094 1.93763

A77 1.94202 -0.00001 0.00284 -0.00141 0.00142 1.94344

A78 1.86132 -0.00020 -0.00413 -0.00003 -0.00417 1.85715

A79 1.89223 -0.00002 0.00047 -0.00016 0.00031 1.89253

A80 1.89223 -0.00002 0.00047 -0.00016 0.00031 1.89253

A81 1.93669 0.00012 0.00005 0.00089 0.00094 1.93763

A82 1.93669 0.00012 0.00005 0.00089 0.00094 1.93763

A83 1.94202 -0.00001 0.00284 -0.00141 0.00142 1.94344

A84 1.86132 -0.00020 -0.00413 -0.00003 -0.00417 1.85715

A85 1.89223 -0.00002 0.00047 -0.00016 0.00031 1.89253

A86 1.89223 -0.00002 0.00047 -0.00016 0.00031 1.89253

A87 1.93770 0.00008 0.00049 0.00007 0.00055 1.93825

A88 1.93770 0.00008 0.00049 0.00007 0.00055 1.93825

A89 1.94154 0.00021 0.00263 0.00122 0.00383 1.94538

A90 1.85980 -0.00028 -0.00478 -0.00130 -0.00608 1.85372

A91 1.89217 -0.00007 0.00045 -0.00008 0.00036 1.89253

A92 1.89217 -0.00007 0.00045 -0.00008 0.00036 1.89253

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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

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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

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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

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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 1.03276 -0.00012 -0.00268 -0.00077 -0.00345 1.02931

D31 -1.03276 0.00012 0.00268 0.00077 0.00345 -1.02931

D32 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

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D34 2.10884 0.00012 0.00268 0.00077 0.00345 2.11228

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D63 1.03306 -0.00005 -0.00255 0.00055 -0.00200 1.03106

D64 -1.03306 0.00005 0.00255 -0.00055 0.00200 -1.03106

D65 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D66 -2.10854 -0.00005 -0.00255 0.00055 -0.00200 -2.11054

D67 2.10854 0.00005 0.00255 -0.00055 0.00200 2.11054

D68 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

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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

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D80 2.10854 0.00005 0.00255 -0.00055 0.00200 2.11054

D81 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

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D83 -1.03306 0.00005 0.00255 -0.00055 0.00200 -1.03106

D84 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

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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

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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

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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

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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 1.03276 -0.00012 -0.00268 -0.00077 -0.00345 1.02931

D126 -1.03276 0.00012 0.00268 0.00077 0.00345 -1.02931

D127 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D128 -2.10884 -0.00012 -0.00268 -0.00077 -0.00345 -2.11228

D129 2.10884 0.00012 0.00268 0.00077 0.00345 2.11228

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 0.004899 0.000450 NO

RMS Force 0.000934 0.000300 NO

Maximum Displacement 0.021608 0.001800 NO

RMS Displacement 0.004519 0.001200 NO

Predicted change in Energy=-5.125223D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 13:53:00 2019, MaxMem= 2415919104 cpu: 1.2

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.084477 -2.189488 0.000000

2 7 0 -0.739300 -1.864878 0.000000

3 6 0 -0.004451 -2.990057 0.000000

4 6 0 -0.934285 -4.155272 0.000000

5 6 0 -2.195944 -3.641139 0.000000

6 7 0 1.337609 -3.117290 0.000000

7 6 0 2.180239 -2.062837 0.000000

8 7 0 1.858799 -0.751881 0.000000

9 6 0 3.011186 0.003858 0.000000

10 6 0 4.166388 -0.919604 0.000000

11 6 0 3.648270 -2.176764 0.000000

12 7 0 -3.114088 -1.332275 0.000000

13 6 0 -4.166388 0.919604 0.000000

14 6 0 -3.648270 2.176764 0.000000

15 6 0 -2.180239 2.062837 0.000000

16 7 0 -1.858799 0.751881 0.000000

17 6 0 -3.011186 -0.003858 0.000000

18 7 0 -1.337609 3.117290 0.000000

19 7 0 0.739300 1.864878 0.000000

20 6 0 0.004451 2.990057 0.000000

21 6 0 0.934285 4.155272 0.000000

22 6 0 2.195944 3.641139 0.000000

23 6 0 2.084477 2.189488 0.000000

24 7 0 3.114088 1.332275 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.482438 -5.571347 0.000000

27 1 0 -3.129460 -4.185767 0.000000

28 6 0 5.587656 -0.482604 0.000000

29 1 0 4.188570 -3.113162 0.000000

30 6 0 -5.587656 0.482604 0.000000

31 1 0 -4.188570 3.113162 0.000000

32 6 0 0.482438 5.571347 0.000000

33 1 0 3.129460 4.185767 0.000000

34 1 0 -1.328290 -6.260201 0.000000

35 1 0 0.138603 -5.785883 0.875273

36 1 0 0.138603 -5.785883 -0.875273

37 1 0 5.808414 0.134207 0.875838

38 1 0 5.808414 0.134207 -0.875838

39 1 0 6.265737 -1.336831 0.000000

40 1 0 -5.808414 -0.134207 0.875838

41 1 0 -5.808414 -0.134207 -0.875838

42 1 0 -6.265737 1.336831 0.000000

43 1 0 -0.138603 5.785883 0.875273

44 1 0 -0.138603 5.785883 -0.875273

45 1 0 1.328290 6.260201 0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.383789 0.000000

3 C 2.228770 1.343886 0.000000

4 C 2.277553 2.298678 1.490743 0.000000

5 C 1.455925 2.297154 2.286165 1.362394 0.000000

6 N 3.545629 2.425301 1.348078 2.497780 3.572172

7 C 4.266596 2.926242 2.373311 3.752138 4.652098

8 N 4.197159 2.826461 2.912239 4.402770 4.978831

9 C 5.547662 4.190265 4.249423 5.732809 6.356116

10 C 6.378552 4.995930 4.656466 6.040398 6.919973

11 C 5.732762 4.398641 3.742168 4.991423 6.024885

12 N 1.339744 2.433780 3.523930 3.566631 2.484722

13 C 3.741765 4.415685 5.710268 6.016715 4.968202

14 C 4.637845 4.979657 6.322457 6.889151 5.996437

15 C 4.253403 4.183689 5.501435 6.341710 5.703998

16 N 2.950014 2.846174 4.176207 4.993483 4.405939

17 C 2.373978 2.936812 4.237669 4.641957 3.727524

18 N 5.359077 5.017965 6.251159 7.283737 6.812717

19 N 4.940810 4.012149 4.911574 6.248447 6.239542

20 C 5.584918 4.911574 5.980120 7.206729 6.986738

21 C 7.026301 6.248447 7.206729 8.518021 8.401331

22 C 7.233134 6.239542 6.986738 8.401331 8.504132

23 C 6.046124 4.940810 5.584918 7.026301 7.233134

24 N 6.279164 5.007034 5.329901 6.819274 7.275390

25 Zn 3.023062 2.006075 2.990060 4.259011 4.252066

26 C 3.742125 3.715359 2.625173 1.486417 2.581047

27 H 2.253246 3.331575 3.345953 2.195387 1.080773

28 C 7.859712 6.476191 6.128538 7.484931 8.400046

29 H 6.340686 5.083515 4.194829 5.227775 6.406308

30 C 4.405944 5.386764 6.575070 6.569913 5.339379

31 H 5.704849 6.056265 7.399739 7.963699 7.042098

32 C 8.174327 7.535920 8.575238 9.829253 9.593938

33 H 8.235838 7.181756 7.830316 9.278305 9.466805

34 H 4.140353 4.434610 3.527944 2.141487 2.759041

35 H 4.317666 4.112310 2.933123 2.139178 3.288789

36 H 4.317666 4.112310 2.933123 2.139178 3.288789

37 H 8.274321 6.901884 6.657141 8.039323 8.893261

38 H 8.274321 6.901884 6.657141 8.039323 8.893261

39 H 8.393634 7.024911 6.484475 7.732006 8.769828

40 H 4.342693 5.427544 6.527553 6.379122 5.110343

41 H 4.342693 5.427544 6.527553 6.379122 5.110343

42 H 5.469722 6.386896 7.610890 7.654252 6.429884

43 H 8.255851 7.724059 8.820500 10.011282 9.688525

44 H 8.255851 7.724059 8.820500 10.011282 9.688525

45 H 9.112860 8.384023 9.345772 10.658392 10.509841

6 7 8 9 10

6 N 0.000000

7 C 1.349776 0.000000

8 N 2.422148 1.349789 0.000000

9 C 3.541529 2.227488 1.378092 0.000000

10 C 3.582153 2.291675 2.313676 1.478943 0.000000

11 C 2.494744 1.472446 2.287466 2.271781 1.359742

12 N 4.796236 5.344494 5.006642 6.269309 7.292162

13 C 6.825723 7.012462 6.252738 7.235756 8.533337

14 C 7.272276 7.207339 6.237369 7.004990 8.405735

15 C 6.261706 6.002912 4.923054 5.584827 7.012462

16 N 5.018715 4.923054 4.010216 4.927098 6.252738

17 C 5.348409 5.584827 4.927098 6.022378 7.235756

18 N 6.784304 6.261706 5.018715 5.348409 6.825723

19 N 5.017965 4.183689 2.846174 2.936812 4.415685

20 C 6.251159 5.501435 4.176207 4.237669 5.710268

21 C 7.283737 6.341710 4.993483 4.641957 6.016715

22 C 6.812717 5.703998 4.405939 3.727524 4.968202

23 C 5.359077 4.253403 2.950014 2.373978 3.741765

24 N 4.791087 3.521202 2.432994 1.332397 2.485617

25 Zn 3.392152 3.001456 2.005108 3.011189 4.266669

26 C 3.055318 4.404485 5.358045 6.579386 6.576496

27 H 4.593076 5.718368 6.055931 7.433740 7.993574

28 C 5.000447 3.756012 3.738567 2.621992 1.486933

29 H 2.850965 2.266402 3.317150 3.331973 2.193670

30 C 7.805032 8.174317 7.548089 8.612159 9.854317

31 H 8.328096 8.206869 7.176993 7.842466 9.277313

32 C 8.730621 7.820697 6.471289 6.114859 7.463507

33 H 7.519666 6.320291 5.098524 4.183582 5.209610

34 H 4.121274 5.470615 6.363892 7.620333 7.662471

35 H 3.053704 4.335372 5.391322 6.522188 6.377290

36 H 3.053704 4.335372 5.391322 6.522188 6.377290

37 H 5.597091 4.331022 4.141462 2.934036 2.138659

38 H 5.597091 4.331022 4.141462 2.934036 2.138659

39 H 5.239893 4.149503 4.445590 3.519879 2.140407

40 H 7.793043 8.264701 7.741755 8.864057 10.043935

41 H 7.793043 8.264701 7.741755 8.864057 10.043935

42 H 8.811927 9.104518 8.388730 9.372199 10.673365

43 H 9.067072 8.230767 6.891884 6.642220 8.016395

44 H 9.067072 8.230767 6.891884 6.642220 8.016395

45 H 9.377495 8.366527 7.032121 6.478732 7.720388

11 12 13 14 15

11 C 0.000000

12 N 6.814885 0.000000

13 C 8.405735 2.485617 0.000000

14 C 8.496630 3.549466 1.359742 0.000000

15 C 7.207339 3.521202 2.291675 1.472446 0.000000

16 N 6.237369 2.432994 2.313676 2.287466 1.349789

17 C 7.004990 1.332397 1.478943 2.271781 2.227488

18 N 7.272276 4.791087 3.582153 2.494744 1.349776

19 N 4.979657 5.007034 4.995930 4.398641 2.926242

20 C 6.322457 5.329901 4.656466 3.742168 2.373311

21 C 6.889151 6.819274 6.040398 4.991423 3.752138

22 C 5.996437 7.275390 6.919973 6.024885 4.652098

23 C 4.637845 6.279164 6.378552 5.732762 4.266596

24 N 3.549466 6.774217 7.292162 6.814885 5.344494

25 Zn 4.248315 3.387108 4.266669 4.248315 3.001456

26 C 5.346582 4.989520 7.463507 8.369930 7.820697

27 H 7.069209 2.853533 5.209610 6.383649 6.320291

28 C 2.575150 8.743128 9.854317 9.611169 8.174317

29 H 1.081094 7.516674 9.277313 9.455125 8.206869

30 C 9.611169 3.067951 1.486933 2.575150 3.756012

31 H 9.455125 4.573447 2.193670 1.081094 2.266402

32 C 8.369930 7.784279 6.576496 5.346582 4.404485

33 H 6.383649 8.332508 7.993574 7.069209 5.718368

34 H 6.437438 5.241519 7.720388 8.750125 8.366527

35 H 5.109756 5.583970 8.016395 8.860602 8.230767

36 H 5.109756 5.583970 8.016395 8.860602 8.230767

37 H 3.282363 9.084532 10.043935 9.714320 8.264701

38 H 3.282363 9.084532 10.043935 9.714320 8.264701

39 H 2.748930 9.379826 10.673365 10.518217 9.104518

40 H 9.714320 3.076012 2.138659 3.282363 4.331022

41 H 9.714320 3.076012 2.138659 3.282363 4.331022

42 H 10.518217 4.130014 2.140407 2.748930 4.149503

43 H 8.860602 7.764521 6.377290 5.109756 4.335372

44 H 8.860602 7.764521 6.377290 5.109756 4.335372

45 H 8.750125 8.796614 7.662471 6.437438 5.470615

16 17 18 19 20

16 N 0.000000

17 C 1.378092 0.000000

18 N 2.422148 3.541529 0.000000

19 N 2.826461 4.190265 2.425301 0.000000

20 C 2.912239 4.249423 1.348078 1.343886 0.000000

21 C 4.402770 5.732809 2.497780 2.298678 1.490743

22 C 4.978831 6.356116 3.572172 2.297154 2.286165

23 C 4.197159 5.547662 3.545629 1.383789 2.228770

24 N 5.006642 6.269309 4.796236 2.433780 3.523930

25 Zn 2.005108 3.011189 3.392152 2.006075 2.990060

26 C 6.471289 6.114859 8.730621 7.535920 8.575238

27 H 5.098524 4.183582 7.519666 7.181756 7.830316

28 C 7.548089 8.612159 7.805032 5.386764 6.575070

29 H 7.176993 7.842466 8.328096 6.056265 7.399739

30 C 3.738567 2.621992 5.000447 6.476191 6.128538

31 H 3.317150 3.331973 2.850965 5.083515 4.194829

32 C 5.358045 6.579386 3.055318 3.715359 2.625173

33 H 6.055931 7.433740 4.593076 3.331575 3.345953

34 H 7.032121 6.478732 9.377495 8.384023 9.345772

35 H 6.891884 6.642220 9.067072 7.724059 8.820500

36 H 6.891884 6.642220 9.067072 7.724059 8.820500

37 H 7.741755 8.864057 7.793043 5.427544 6.527553

38 H 7.741755 8.864057 7.793043 5.427544 6.527553

39 H 8.388730 9.372199 8.811927 6.386896 7.610890

40 H 4.141462 2.934036 5.597091 6.901884 6.657141

41 H 4.141462 2.934036 5.597091 6.901884 6.657141

42 H 4.445590 3.519879 5.239893 7.024911 6.484475

43 H 5.391322 6.522188 3.053704 4.112310 2.933123

44 H 5.391322 6.522188 3.053704 4.112310 2.933123

45 H 6.363892 7.620333 4.121274 4.434610 3.527944

21 22 23 24 25

21 C 0.000000

22 C 1.362394 0.000000

23 C 2.277553 1.455925 0.000000

24 N 3.566631 2.484722 1.339744 0.000000

25 Zn 4.259011 4.252066 3.023062 3.387108 0.000000

26 C 9.829253 9.593938 8.174327 7.784279 5.592196

27 H 9.278305 9.466805 8.235838 8.332508 5.226296

28 C 6.569913 5.339379 4.405944 3.067951 5.608458

29 H 7.963699 7.042098 5.704849 4.573447 5.218802

30 C 7.484931 8.400046 7.859712 8.743128 5.608458

31 H 5.227775 6.406308 6.340686 7.516674 5.218802

32 C 1.486417 2.581047 3.742125 4.989520 5.592196

33 H 2.195387 1.080773 2.253246 2.853533 5.226296

34 H 10.658392 10.509841 9.112860 8.796614 6.399568

35 H 10.011282 9.688525 8.255851 7.764521 5.853354

36 H 10.011282 9.688525 8.255851 7.764521 5.853354

37 H 6.379122 5.110343 4.342693 3.076012 5.875609

38 H 6.379122 5.110343 4.342693 3.076012 5.875609

39 H 7.654252 6.429884 5.469722 4.130014 6.406760

40 H 8.039323 8.893261 8.274321 9.084532 5.875609

41 H 8.039323 8.893261 8.274321 9.084532 5.875609

42 H 7.732006 8.769828 8.393634 9.379826 6.406760

43 H 2.139178 3.288789 4.317666 5.583970 5.853354

44 H 2.139178 3.288789 4.317666 5.583970 5.853354

45 H 2.141487 2.759041 4.140353 5.241519 6.399568

26 27 28 29 30

26 C 0.000000

27 H 2.987734 0.000000

28 C 7.920943 9.471089 0.000000

29 H 5.278352 7.396219 2.979475 0.000000

30 C 7.919191 5.276023 11.216917 10.416532 0.000000

31 H 9.442252 7.375370 10.416532 10.437605 2.979475

32 C 11.184392 10.404186 7.919191 9.442252 7.920943

33 H 10.404186 10.452591 5.276023 7.375370 9.471089

34 H 1.090864 2.747269 9.011710 6.351346 7.975438

35 H 1.094449 3.742553 7.653956 4.930698 8.535225

36 H 1.094449 3.742553 7.653956 4.930698 8.535225

37 H 8.537873 9.965685 1.093748 3.733148 11.434985

38 H 8.537873 9.965685 1.093748 3.733148 11.434985

39 H 7.966742 9.817645 1.090641 2.733124 11.992217

40 H 7.661306 4.935486 11.434985 10.468093 1.093748

41 H 7.661306 4.935486 11.434985 10.468093 1.093748

42 H 9.009410 6.351010 11.992217 11.361997 1.090641

43 H 11.396096 10.447255 8.535225 9.933958 7.653956

44 H 11.396096 10.447255 8.535225 9.933958 7.653956

45 H 11.969305 11.357367 7.975438 9.800058 9.011710

31 32 33 34 35

31 H 0.000000

32 C 5.278352 0.000000

33 H 7.396219 2.987734 0.000000

34 H 9.800058 11.969305 11.357367 0.000000

35 H 9.933958 11.396096 10.447255 1.772809 0.000000

36 H 9.933958 11.396096 10.447255 1.772809 1.750545

37 H 10.468093 7.661306 4.935486 9.622271 8.197209

38 H 10.468093 7.661306 4.935486 9.622271 8.382161

39 H 11.361997 9.009410 6.351010 9.050348 7.622462

40 H 3.733148 8.537873 9.965685 7.639791 8.204173

41 H 3.733148 8.537873 9.965685 7.639791 8.388971

42 H 2.733124 7.966742 9.817645 9.060534 9.618457

43 H 4.930698 1.094449 3.742553 12.136292 11.575086

44 H 4.930698 1.094449 3.742553 12.136292 11.706708

45 H 6.351346 1.090864 2.747269 12.799135 12.136292

36 37 38 39 40

36 H 0.000000

37 H 8.382161 0.000000

38 H 8.197209 1.751677 0.000000

39 H 7.622462 1.772059 1.772059 0.000000

40 H 8.388971 11.619929 11.751218 12.165464 0.000000

41 H 8.204173 11.751218 11.619929 12.165464 1.751677

42 H 9.618457 12.165464 12.165464 12.813520 1.772059

43 H 11.706708 8.204173 8.388971 9.618457 8.197209

44 H 11.575086 8.388971 8.204173 9.618457 8.382161

45 H 12.136292 7.639791 7.639791 9.060534 9.622271

41 42 43 44 45

41 H 0.000000

42 H 1.772059 0.000000

43 H 8.382161 7.622462 0.000000

44 H 8.197209 7.622462 1.750545 0.000000

45 H 9.622271 9.050348 1.772809 1.772809 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=3 Diff= 4.37D-03

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 -2.811368 1.111356 0.000000

2 7 0 -2.006026 -0.013942 0.000000

3 6 0 -2.773547 -1.117093 0.000000

4 6 0 -4.202410 -0.692044 0.000000

5 6 0 -4.198893 0.670346 0.000000

6 7 0 -2.388247 -2.408936 0.000000

7 6 0 -1.094764 -2.794679 0.000000

8 7 0 0.000000 -2.005108 0.000000

9 6 0 1.132719 -2.790019 0.000000

10 6 0 0.709822 -4.207210 0.000000

11 6 0 -0.649891 -4.198312 0.000000

12 7 0 -2.402791 2.387279 0.000000

13 6 0 -0.709822 4.207210 0.000000

14 6 0 0.649891 4.198312 0.000000

15 6 0 1.094764 2.794679 0.000000

16 7 0 0.000000 2.005108 0.000000

17 6 0 -1.132719 2.790019 0.000000

18 7 0 2.388247 2.408936 0.000000

19 7 0 2.006026 0.013942 0.000000

20 6 0 2.773547 1.117093 0.000000

21 6 0 4.202410 0.692044 0.000000

22 6 0 4.198893 -0.670346 0.000000

23 6 0 2.811368 -1.111356 0.000000

24 7 0 2.402791 -2.387279 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -5.345722 -1.641924 0.000000

27 1 0 -5.053833 1.331519 0.000000

28 6 0 1.647885 -5.360903 0.000000

29 1 0 -1.315358 -5.050320 0.000000

30 6 0 -1.647885 5.360903 0.000000

31 1 0 1.315358 5.050320 0.000000

32 6 0 5.345722 1.641924 0.000000

33 1 0 5.053833 -1.331519 0.000000

34 1 0 -6.301491 -1.116100 0.000000

35 1 0 -5.311724 -2.298095 0.875273

36 1 0 -5.311724 -2.298095 -0.875273

37 1 0 2.302469 -5.334259 0.875838

38 1 0 2.302469 -5.334259 -0.875838

39 1 0 1.110258 -6.309826 0.000000

40 1 0 -2.302469 5.334259 0.875838

41 1 0 -2.302469 5.334259 -0.875838

42 1 0 -1.110258 6.309826 0.000000

43 1 0 5.311724 2.298095 0.875273

44 1 0 5.311724 2.298095 -0.875273

45 1 0 6.301491 1.116100 0.000000

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

Rotational constants (GHZ): 0.1829799 0.1819121 0.0914262

Leave Link 202 at Tue Sep 17 13:53:00 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 101 beta electrons

nuclear repulsion energy 2761.8386375118 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= -0.1142547041 Hartrees.

Nuclear repulsion after empirical dispersion term = 2761.7243828077 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 = 3490

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.12D-09

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 130

GePol: Fraction of low-weight points (<1% of avg) = 3.72%

GePol: Cavity surface area = 382.016 Ang\*\*2

GePol: Cavity volume = 379.265 Ang\*\*3

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

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

PCM non-electrostatic energy = -0.0107209087 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2761.7136618990 Hartrees.

Leave Link 301 at Tue Sep 17 13:53:00 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= 15327 LenP2D= 41268.

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 13:53:01 2019, MaxMem= 2415919104 cpu: 11.4

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 13:53:01 2019, MaxMem= 2415919104 cpu: 1.2

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= -0.000000 0.000000 -0.000000

Rot= 0.999999 -0.000000 0.000000 -0.001362 Ang= -0.16 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 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0419 S= 1.0139

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= -1276.14741763458

Leave Link 401 at Tue Sep 17 13:53:03 2019, MaxMem= 2415919104 cpu: 40.7

(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 9.21D-15 for 3489.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.47D-15 for 2270 2136.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.55D-15 for 3489.

Iteration 1 A^-1\*A deviation from orthogonality is 2.28D-08 for 2518 2475.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.55D-15 for 272.

Iteration 2 A\*A^-1 deviation from orthogonality is 2.22D-15 for 2508 242.

Iteration 2 A^-1\*A deviation from unit magnitude is 8.88D-16 for 179.

Iteration 2 A^-1\*A deviation from orthogonality is 3.33D-16 for 2518 208.

E= -1275.84001179363

DIIS: error= 7.60D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.84001179363 IErMin= 1 ErrMin= 7.60D-04

ErrMax= 7.60D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.54D-03 BMatP= 1.54D-03

IDIUse=3 WtCom= 9.92D-01 WtEn= 7.60D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.298 Goal= None Shift= 0.000

Gap= 0.397 Goal= None Shift= 0.000

RMSDP=5.75D-05 MaxDP=1.75D-03 OVMax= 1.58D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 5.75D-05 CP: 1.00D+00

E= -1275.84056894239 Delta-E= -0.000557148760 Rises=F Damp=F

DIIS: error= 4.44D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84056894239 IErMin= 2 ErrMin= 4.44D-04

ErrMax= 4.44D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.95D-04 BMatP= 1.54D-03

IDIUse=3 WtCom= 9.96D-01 WtEn= 4.44D-03

Coeff-Com: 0.128D+00 0.872D+00

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

Coeff: 0.127D+00 0.873D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=2.19D-05 MaxDP=1.10D-03 DE=-5.57D-04 OVMax= 4.84D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.19D-05 CP: 1.00D+00 1.02D+00

E= -1275.84054967334 Delta-E= 0.000019269046 Rises=F Damp=F

DIIS: error= 7.33D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1275.84056894239 IErMin= 2 ErrMin= 4.44D-04

ErrMax= 7.33D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.26D-04 BMatP= 1.95D-04

IDIUse=3 WtCom= 2.70D-01 WtEn= 7.30D-01

Coeff-Com: -0.194D-01 0.575D+00 0.444D+00

Coeff-En: 0.000D+00 0.575D+00 0.425D+00

Coeff: -0.524D-02 0.575D+00 0.430D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=1.59D-05 MaxDP=6.93D-04 DE= 1.93D-05 OVMax= 3.40D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 9.75D-06 CP: 1.00D+00 1.10D+00 4.67D-01

E= -1275.84062549191 Delta-E= -0.000075818572 Rises=F Damp=F

DIIS: error= 1.20D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84062549191 IErMin= 4 ErrMin= 1.20D-04

ErrMax= 1.20D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.79D-06 BMatP= 1.95D-04

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.20D-03

Coeff-Com: -0.134D-01 0.186D+00 0.205D+00 0.623D+00

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

Coeff: -0.134D-01 0.186D+00 0.204D+00 0.623D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=5.52D-06 MaxDP=1.74D-04 DE=-7.58D-05 OVMax= 2.90D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.23D-06 CP: 1.00D+00 1.11D+00 6.12D-01 1.14D+00

E= -1275.84063039893 Delta-E= -0.000004907019 Rises=F Damp=F

DIIS: error= 6.88D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84063039893 IErMin= 5 ErrMin= 6.88D-05

ErrMax= 6.88D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.99D-06 BMatP= 9.79D-06

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

Coeff-Com: -0.236D-02-0.125D-01 0.349D-01 0.363D+00 0.617D+00

Coeff: -0.236D-02-0.125D-01 0.349D-01 0.363D+00 0.617D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=4.09D-06 MaxDP=1.50D-04 DE=-4.91D-06 OVMax= 2.84D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.73D-06 CP: 1.00D+00 1.13D+00 6.62D-01 1.47D+00 1.24D+00

E= -1275.84063310118 Delta-E= -0.000002702247 Rises=F Damp=F

DIIS: error= 5.85D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84063310118 IErMin= 6 ErrMin= 5.85D-05

ErrMax= 5.85D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.80D-07 BMatP= 2.99D-06

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

Coeff-Com: 0.426D-02-0.675D-01-0.527D-01-0.132D+00 0.261D-01 0.122D+01

Coeff: 0.426D-02-0.675D-01-0.527D-01-0.132D+00 0.261D-01 0.122D+01

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=6.33D-06 MaxDP=2.37D-04 DE=-2.70D-06 OVMax= 4.69D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.18D-06 CP: 1.00D+00 1.15D+00 7.61D-01 1.90D+00 1.95D+00

CP: 2.24D+00

E= -1275.84063544222 Delta-E= -0.000002341044 Rises=F Damp=F

DIIS: error= 4.33D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84063544222 IErMin= 7 ErrMin= 4.33D-05

ErrMax= 4.33D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.66D-07 BMatP= 5.80D-07

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

Coeff-Com: 0.379D-02-0.447D-01-0.504D-01-0.233D+00-0.229D+00 0.880D+00

Coeff-Com: 0.673D+00

Coeff: 0.379D-02-0.447D-01-0.504D-01-0.233D+00-0.229D+00 0.880D+00

Coeff: 0.673D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=4.40D-06 MaxDP=1.65D-04 DE=-2.34D-06 OVMax= 3.36D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 8.73D-07 CP: 1.00D+00 1.17D+00 8.25D-01 2.20D+00 2.45D+00

CP: 3.00D+00 1.43D+00

E= -1275.84063646989 Delta-E= -0.000001027665 Rises=F Damp=F

DIIS: error= 3.05D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84063646989 IErMin= 8 ErrMin= 3.05D-05

ErrMax= 3.05D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.19D-07 BMatP= 4.66D-07

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

Coeff-Com: -0.863D-03 0.242D-01 0.153D-01 0.619D-02-0.800D-01-0.345D+00

Coeff-Com: 0.270D+00 0.111D+01

Coeff: -0.863D-03 0.242D-01 0.153D-01 0.619D-02-0.800D-01-0.345D+00

Coeff: 0.270D+00 0.111D+01

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=4.05D-06 MaxDP=1.61D-04 DE=-1.03D-06 OVMax= 3.22D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.38D-06 CP: 1.00D+00 1.18D+00 8.74D-01 2.45D+00 2.92D+00

CP: 3.00D+00 2.29D+00 2.69D+00

E= -1275.84063702054 Delta-E= -0.000000550652 Rises=F Damp=F

DIIS: error= 1.93D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84063702054 IErMin= 9 ErrMin= 1.93D-05

ErrMax= 1.93D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.92D-08 BMatP= 1.19D-07

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

Coeff-Com: -0.144D-02 0.233D-01 0.219D-01 0.669D-01 0.335D-01-0.399D+00

Coeff-Com: -0.544D-01 0.539D+00 0.771D+00

Coeff: -0.144D-02 0.233D-01 0.219D-01 0.669D-01 0.335D-01-0.399D+00

Coeff: -0.544D-01 0.539D+00 0.771D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=1.90D-06 MaxDP=7.51D-05 DE=-5.51D-07 OVMax= 1.53D-03

Cycle 10 Pass 1 IDiag 1:

RMSU= 8.62D-07 CP: 1.00D+00 1.18D+00 8.97D-01 2.55D+00 3.00D+00

CP: 3.00D+00 2.74D+00 3.00D+00 1.43D+00

E= -1275.84063719053 Delta-E= -0.000000169996 Rises=F Damp=F

DIIS: error= 1.38D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84063719053 IErMin=10 ErrMin= 1.38D-05

ErrMax= 1.38D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.23D-08 BMatP= 4.92D-08

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

Coeff-Com: -0.104D-03-0.387D-02 0.145D-02 0.254D-01 0.609D-01-0.192D-02

Coeff-Com: -0.181D+00-0.305D+00 0.343D+00 0.106D+01

Coeff: -0.104D-03-0.387D-02 0.145D-02 0.254D-01 0.609D-01-0.192D-02

Coeff: -0.181D+00-0.305D+00 0.343D+00 0.106D+01

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=2.04D-06 MaxDP=8.04D-05 DE=-1.70D-07 OVMax= 1.65D-03

Cycle 11 Pass 1 IDiag 1:

RMSU= 4.06D-07 CP: 1.00D+00 1.19D+00 9.21D-01 2.66D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.93D+00 2.54D+00

E= -1275.84063731498 Delta-E= -0.000000124447 Rises=F Damp=F

DIIS: error= 8.66D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84063731498 IErMin=11 ErrMin= 8.66D-06

ErrMax= 8.66D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.14D-09 BMatP= 2.23D-08

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

Coeff-Com: 0.485D-03-0.108D-01-0.741D-02-0.108D-01 0.140D-01 0.156D+00

Coeff-Com: -0.776D-01-0.323D+00-0.155D+00 0.447D+00 0.967D+00

Coeff: 0.485D-03-0.108D-01-0.741D-02-0.108D-01 0.140D-01 0.156D+00

Coeff: -0.776D-01-0.323D+00-0.155D+00 0.447D+00 0.967D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=1.37D-06 MaxDP=5.46D-05 DE=-1.24D-07 OVMax= 1.10D-03

Cycle 12 Pass 1 IDiag 1:

RMSU= 5.58D-07 CP: 1.00D+00 1.19D+00 9.36D-01 2.74D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.25D+00 3.00D+00

CP: 1.93D+00

E= -1275.84063736668 Delta-E= -0.000000051703 Rises=F Damp=F

DIIS: error= 4.93D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84063736668 IErMin=12 ErrMin= 4.93D-06

ErrMax= 4.93D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.74D-09 BMatP= 9.14D-09

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

Coeff-Com: 0.324D-03-0.367D-02-0.484D-02-0.195D-01-0.326D-01 0.885D-01

Coeff-Com: 0.554D-01 0.236D-01-0.298D+00-0.454D+00 0.592D+00 0.105D+01

Coeff: 0.324D-03-0.367D-02-0.484D-02-0.195D-01-0.326D-01 0.885D-01

Coeff: 0.554D-01 0.236D-01-0.298D+00-0.454D+00 0.592D+00 0.105D+01

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=1.31D-06 MaxDP=5.19D-05 DE=-5.17D-08 OVMax= 1.05D-03

Cycle 13 Pass 1 IDiag 1:

RMSU= 2.25D-07 CP: 1.00D+00 1.19D+00 9.50D-01 2.81D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.56D+00 3.00D+00

CP: 2.85D+00 2.53D+00

E= -1275.84063739184 Delta-E= -0.000000025153 Rises=F Damp=F

DIIS: error= 1.69D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84063739184 IErMin=13 ErrMin= 1.69D-06

ErrMax= 1.69D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.67D-10 BMatP= 4.74D-09

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

Coeff-Com: -0.191D-04 0.204D-02 0.682D-03-0.347D-02-0.175D-01-0.184D-01

Coeff-Com: 0.435D-01 0.110D+00-0.516D-01-0.310D+00-0.629D-01 0.370D+00

Coeff-Com: 0.938D+00

Coeff: -0.191D-04 0.204D-02 0.682D-03-0.347D-02-0.175D-01-0.184D-01

Coeff: 0.435D-01 0.110D+00-0.516D-01-0.310D+00-0.629D-01 0.370D+00

Coeff: 0.938D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=5.15D-07 MaxDP=2.07D-05 DE=-2.52D-08 OVMax= 4.16D-04

Cycle 14 Pass 1 IDiag 1:

RMSU= 1.15D-07 CP: 1.00D+00 1.19D+00 9.56D-01 2.84D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.68D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.29D+00

E= -1275.84063739479 Delta-E= -0.000000002952 Rises=F Damp=F

DIIS: error= 3.16D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84063739479 IErMin=14 ErrMin= 3.16D-07

ErrMax= 3.16D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.57D-10 BMatP= 6.67D-10

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

Coeff-Com: -0.480D-04 0.145D-02 0.956D-03 0.692D-03-0.480D-02-0.191D-01

Coeff-Com: 0.164D-01 0.496D-01 0.632D-02-0.107D+00-0.935D-01 0.708D-01

Coeff-Com: 0.467D+00 0.611D+00

Coeff: -0.480D-04 0.145D-02 0.956D-03 0.692D-03-0.480D-02-0.191D-01

Coeff: 0.164D-01 0.496D-01 0.632D-02-0.107D+00-0.935D-01 0.708D-01

Coeff: 0.467D+00 0.611D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=7.59D-08 MaxDP=2.91D-06 DE=-2.95D-09 OVMax= 6.01D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 3.00D-08 CP: 1.00D+00 1.19D+00 9.57D-01 2.84D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.70D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.34D+00 1.42D+00

E= -1275.84063739494 Delta-E= -0.000000000153 Rises=F Damp=F

DIIS: error= 1.59D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.84063739494 IErMin=15 ErrMin= 1.59D-07

ErrMax= 1.59D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.70D-11 BMatP= 1.57D-10

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

Coeff-Com: -0.214D-04 0.277D-03 0.363D-03 0.134D-02 0.209D-02-0.613D-02

Coeff-Com: -0.164D-02-0.192D-02 0.176D-01 0.214D-01-0.380D-01-0.587D-01

Coeff-Com: 0.226D-01 0.332D+00 0.709D+00

Coeff: -0.214D-04 0.277D-03 0.363D-03 0.134D-02 0.209D-02-0.613D-02

Coeff: -0.164D-02-0.192D-02 0.176D-01 0.214D-01-0.380D-01-0.587D-01

Coeff: 0.226D-01 0.332D+00 0.709D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=2.96D-08 MaxDP=1.23D-06 DE=-1.53D-10 OVMax= 2.28D-05

Cycle 16 Pass 1 IDiag 1:

RMSU= 8.64D-09 CP: 1.00D+00 1.19D+00 9.57D-01 2.84D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.71D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.36D+00 1.59D+00 1.30D+00

E= -1275.84063739496 Delta-E= -0.000000000021 Rises=F Damp=F

DIIS: error= 7.99D-08 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1275.84063739496 IErMin=16 ErrMin= 7.99D-08

ErrMax= 7.99D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.81D-12 BMatP= 3.70D-11

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

Coeff-Com: -0.312D-05-0.123D-03 0.268D-05 0.583D-03 0.211D-02 0.225D-03

Coeff-Com: -0.385D-02-0.103D-01 0.817D-02 0.324D-01-0.323D-02-0.467D-01

Coeff-Com: -0.757D-01 0.514D-01 0.402D+00 0.642D+00

Coeff: -0.312D-05-0.123D-03 0.268D-05 0.583D-03 0.211D-02 0.225D-03

Coeff: -0.385D-02-0.103D-01 0.817D-02 0.324D-01-0.323D-02-0.467D-01

Coeff: -0.757D-01 0.514D-01 0.402D+00 0.642D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=8.29D-09 MaxDP=3.27D-07 DE=-2.14D-11 OVMax= 5.69D-06

Error on total polarization charges = 0.06463

SCF Done: E(UB3LYP) = -1275.84063739 A.U. after 16 cycles

NFock= 16 Conv=0.83D-08 -V/T= 1.9659

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0426 S= 1.0141

<L.S>= 0.000000000000E+00

KE= 1.320818537530D+03 PE=-8.575375637196D+03 EE= 3.217002800373D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.73

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0426, after 2.0011

Leave Link 502 at Tue Sep 17 13:54:35 2019, MaxMem= 2415919104 cpu: 1615.5

(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= 15327 LenP2D= 41268.

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 = 246

Leave Link 701 at Tue Sep 17 13:54:39 2019, MaxMem= 2415919104 cpu: 69.7

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 13:54:39 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 13:54:52 2019, MaxMem= 2415919104 cpu: 225.5

(Enter /home/blab/g09/l716.exe)

Dipole = 3.44613227D-13-1.13242749D-13-2.22044605D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000967295 -0.002270470 0.000000000

2 7 0.001712992 -0.000391210 0.000000000

3 6 -0.002860278 0.000344097 0.000000000

4 6 0.001750071 -0.001015886 0.000000000

5 6 -0.000621442 0.002005380 -0.000000000

6 7 0.002434613 0.001033492 -0.000000000

7 6 -0.001502843 -0.000009482 0.000000000

8 7 -0.000599363 -0.001286460 -0.000000000

9 6 0.001138939 0.002385892 0.000000000

10 6 -0.000346496 -0.000407933 0.000000000

11 6 0.000770851 -0.000424721 -0.000000000

12 7 0.000814845 0.002830183 -0.000000000

13 6 0.000346496 0.000407933 -0.000000000

14 6 -0.000770851 0.000424721 0.000000000

15 6 0.001502843 0.000009482 0.000000000

16 7 0.000599363 0.001286460 -0.000000000

17 6 -0.001138939 -0.002385892 0.000000000

18 7 -0.002434613 -0.001033492 0.000000000

19 7 -0.001712992 0.000391210 -0.000000000

20 6 0.002860278 -0.000344097 0.000000000

21 6 -0.001750071 0.001015886 0.000000000

22 6 0.000621442 -0.002005380 -0.000000000

23 6 0.000967295 0.002270470 -0.000000000

24 7 -0.000814845 -0.002830183 0.000000000

25 30 -0.000000000 0.000000000 0.000000000

26 6 -0.000239854 0.000211757 0.000000000

27 1 -0.000271126 -0.000125551 -0.000000000

28 6 0.000152865 0.000096775 -0.000000000

29 1 -0.000059874 -0.000122474 0.000000000

30 6 -0.000152865 -0.000096775 0.000000000

31 1 0.000059874 0.000122474 -0.000000000

32 6 0.000239854 -0.000211757 0.000000000

33 1 0.000271126 0.000125551 0.000000000

34 1 -0.000192655 -0.000162711 0.000000000

35 1 0.000200001 -0.000040687 0.000548620

36 1 0.000200001 -0.000040687 -0.000548620

37 1 0.000084470 0.000221209 0.000575660

38 1 0.000084470 0.000221209 -0.000575660

39 1 0.000151777 -0.000219685 0.000000000

40 1 -0.000084470 -0.000221209 0.000575660

41 1 -0.000084470 -0.000221209 -0.000575660

42 1 -0.000151777 0.000219685 -0.000000000

43 1 -0.000200001 0.000040687 0.000548620

44 1 -0.000200001 0.000040687 -0.000548620

45 1 0.000192655 0.000162711 -0.000000000

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

Cartesian Forces: Max 0.002860278 RMS 0.000909303

Leave Link 716 at Tue Sep 17 13:54:52 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 0.001797443 RMS 0.000366934

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= -5.96D-04 DEPred=-5.13D-04 R= 1.16D+00

TightC=F SS= 1.41D+00 RLast= 6.98D-02 DXNew= 5.0454D-01 2.0947D-01

Trust test= 1.16D+00 RLast= 6.98D-02 DXMaxT set to 3.00D-01

ITU= 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01338

Eigenvalues --- 0.01340 0.01344 0.01345 0.01604 0.01622

Eigenvalues --- 0.01635 0.01637 0.01775 0.01791 0.01815

Eigenvalues --- 0.01816 0.01892 0.01908 0.01943 0.01947

Eigenvalues --- 0.01998 0.01999 0.02044 0.02049 0.02070

Eigenvalues --- 0.02088 0.02102 0.02112 0.02113 0.02205

Eigenvalues --- 0.02311 0.02317 0.02350 0.02373 0.07177

Eigenvalues --- 0.07177 0.07199 0.07199 0.07323 0.07347

Eigenvalues --- 0.07350 0.07368 0.14493 0.14505 0.15078

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 0.16011 0.16048

Eigenvalues --- 0.16414 0.17139 0.18477 0.22067 0.22085

Eigenvalues --- 0.23842 0.23852 0.23878 0.24160 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25112

Eigenvalues --- 0.27537 0.31367 0.33193 0.33197 0.33243

Eigenvalues --- 0.33282 0.33282 0.33316 0.33338 0.33724

Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.34321 0.34371 0.34437 0.34437

Eigenvalues --- 0.34439 0.35469 0.35549 0.35563 0.35606

Eigenvalues --- 0.35682 0.35682 0.35748 0.36639 0.38874

Eigenvalues --- 0.39728 0.41711 0.41735 0.44753 0.47928

Eigenvalues --- 0.48941 0.49006 0.50007 0.50743 0.51359

Eigenvalues --- 0.51360 0.52470 0.54015 0.54035 0.54380

Eigenvalues --- 0.56307 0.56340 0.56398 0.59833

DIIS coeff's: 1.31654 -0.43303 0.11648

Cosine: 0.997 > 0.840

Length: 1.109

GDIIS step was calculated using 3 of the last 3 vectors.

Iteration 1 RMS(Cart)= 0.00148708 RMS(Int)= 0.00000269

Iteration 2 RMS(Cart)= 0.00000425 RMS(Int)= 0.00000199

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000199

ITry= 1 IFail=0 DXMaxC= 6.45D-03 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 3.87D-10 for atom 38.

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

(Linear) (Quad) (Total)

R1 2.61498 0.00060 0.00279 0.00128 0.00407 2.61906

R2 2.75130 -0.00099 -0.00097 -0.00322 -0.00419 2.74711

R3 2.53175 0.00065 0.00049 0.00053 0.00102 2.53277

R4 2.53958 -0.00073 -0.00329 -0.00083 -0.00413 2.53545

R5 3.79093 0.00015 0.00181 -0.00044 0.00137 3.79230

R6 2.81710 -0.00019 0.00235 -0.00136 0.00099 2.81808

R7 2.54750 0.00153 0.00177 0.00274 0.00451 2.55201

R8 2.57455 0.00149 0.00023 0.00273 0.00296 2.57751

R9 2.80892 0.00002 0.00001 -0.00066 -0.00065 2.80827

R10 2.04237 0.00030 0.00016 0.00065 0.00081 2.04318

R11 2.55071 -0.00127 0.00082 -0.00289 -0.00207 2.54864

R12 2.55073 -0.00054 -0.00265 -0.00070 -0.00335 2.54738

R13 2.78252 0.00072 0.00201 0.00185 0.00386 2.78638

R14 2.60422 0.00062 0.00210 0.00132 0.00342 2.60763

R15 3.78911 0.00015 0.00140 -0.00132 0.00009 3.78919

R16 2.79480 0.00030 0.00095 0.00041 0.00136 2.79616

R17 2.51787 -0.00180 -0.00092 -0.00424 -0.00516 2.51270

R18 2.56954 0.00020 -0.00065 0.00000 -0.00065 2.56889

R19 2.80990 0.00054 0.00020 0.00126 0.00146 2.81136

R20 2.04297 0.00008 0.00052 -0.00050 0.00002 2.04299

R21 2.51787 -0.00180 -0.00092 -0.00424 -0.00516 2.51270

R22 2.56954 0.00020 -0.00065 0.00000 -0.00065 2.56889

R23 2.79480 0.00030 0.00095 0.00041 0.00136 2.79616

R24 2.80990 0.00054 0.00020 0.00126 0.00146 2.81136

R25 2.78252 0.00072 0.00201 0.00185 0.00386 2.78638

R26 2.04297 0.00008 0.00052 -0.00050 0.00002 2.04299

R27 2.55073 -0.00054 -0.00265 -0.00070 -0.00335 2.54738

R28 2.55071 -0.00127 0.00082 -0.00289 -0.00207 2.54864

R29 2.60422 0.00062 0.00210 0.00132 0.00342 2.60763

R30 3.78911 0.00015 0.00140 -0.00132 0.00009 3.78919

R31 2.54750 0.00153 0.00177 0.00274 0.00451 2.55201

R32 2.53958 -0.00073 -0.00329 -0.00083 -0.00413 2.53545

R33 2.61498 0.00060 0.00279 0.00128 0.00407 2.61906

R34 3.79093 0.00015 0.00181 -0.00044 0.00137 3.79230

R35 2.81710 -0.00019 0.00235 -0.00136 0.00099 2.81808

R36 2.57455 0.00149 0.00023 0.00273 0.00296 2.57751

R37 2.80892 0.00002 0.00001 -0.00066 -0.00065 2.80827

R38 2.75130 -0.00099 -0.00097 -0.00322 -0.00419 2.74711

R39 2.04237 0.00030 0.00016 0.00065 0.00081 2.04318

R40 2.53175 0.00065 0.00049 0.00053 0.00102 2.53277

R41 2.06143 0.00025 0.00030 0.00029 0.00059 2.06202

R42 2.06821 0.00056 0.00071 0.00065 0.00136 2.06957

R43 2.06821 0.00056 0.00071 0.00065 0.00136 2.06957

R44 2.06688 0.00060 0.00068 0.00075 0.00143 2.06831

R45 2.06688 0.00060 0.00068 0.00075 0.00143 2.06831

R46 2.06101 0.00027 0.00021 0.00041 0.00062 2.06163

R47 2.06688 0.00060 0.00068 0.00075 0.00143 2.06831

R48 2.06688 0.00060 0.00068 0.00075 0.00143 2.06831

R49 2.06101 0.00027 0.00021 0.00041 0.00062 2.06163

R50 2.06821 0.00056 0.00071 0.00065 0.00136 2.06957

R51 2.06821 0.00056 0.00071 0.00065 0.00136 2.06957

R52 2.06143 0.00025 0.00030 0.00029 0.00059 2.06202

A1 1.88422 0.00002 -0.00109 0.00060 -0.00049 1.88373

A2 2.21052 -0.00057 -0.00170 -0.00111 -0.00280 2.20772

A3 2.18844 0.00056 0.00279 0.00051 0.00329 2.19174

A4 1.91256 -0.00000 0.00020 -0.00028 -0.00009 1.91247

A5 2.18501 -0.00038 -0.00091 -0.00109 -0.00200 2.18301

A6 2.18562 0.00038 0.00071 0.00137 0.00209 2.18771

A7 1.88953 0.00045 0.00114 0.00023 0.00137 1.89090

A8 2.24387 -0.00051 0.00055 -0.00107 -0.00052 2.24334

A9 2.14979 0.00006 -0.00169 0.00084 -0.00085 2.14894

A10 1.85735 -0.00058 -0.00181 -0.00017 -0.00199 1.85537

A11 2.15921 0.00032 -0.00034 0.00042 0.00008 2.15929

A12 2.26663 0.00026 0.00215 -0.00025 0.00190 2.26853

A13 1.88112 0.00011 0.00156 -0.00037 0.00120 1.88232

A14 2.17557 -0.00009 -0.00116 0.00021 -0.00095 2.17462

A15 2.22650 -0.00003 -0.00041 0.00016 -0.00025 2.22625

A16 2.15048 0.00009 -0.00134 -0.00083 -0.00218 2.14829

A17 2.22694 0.00007 0.00054 0.00064 0.00117 2.22811

A18 2.16755 -0.00033 -0.00169 -0.00025 -0.00194 2.16561

A19 1.88870 0.00026 0.00116 -0.00039 0.00076 1.88946

A20 1.91079 -0.00006 0.00004 0.00008 0.00011 1.91090

A21 2.19563 0.00033 0.00077 0.00113 0.00190 2.19753

A22 2.17677 -0.00026 -0.00081 -0.00121 -0.00202 2.17476

A23 1.88678 0.00000 -0.00096 0.00033 -0.00063 1.88615

A24 2.22855 -0.00023 -0.00111 0.00027 -0.00084 2.22771

A25 2.16786 0.00023 0.00207 -0.00060 0.00147 2.16933

A26 1.85425 0.00001 0.00094 -0.00052 0.00042 1.85467

A27 2.16892 -0.00021 -0.00117 -0.00057 -0.00174 2.16718

A28 2.26002 0.00020 0.00023 0.00109 0.00132 2.26134

A29 1.88427 -0.00020 -0.00117 0.00050 -0.00067 1.88360

A30 2.17158 -0.00001 -0.00016 -0.00070 -0.00087 2.17071

A31 2.22734 0.00022 0.00134 0.00020 0.00154 2.22888

A32 2.18777 0.00109 0.00330 0.00189 0.00520 2.19297

A33 1.85425 0.00001 0.00094 -0.00052 0.00042 1.85467

A34 2.26002 0.00020 0.00023 0.00109 0.00132 2.26134

A35 2.16892 -0.00021 -0.00117 -0.00057 -0.00174 2.16718

A36 1.88427 -0.00020 -0.00117 0.00050 -0.00067 1.88360

A37 2.22734 0.00022 0.00134 0.00020 0.00154 2.22888

A38 2.17158 -0.00001 -0.00016 -0.00070 -0.00087 2.17071

A39 1.88870 0.00026 0.00116 -0.00039 0.00076 1.88946

A40 2.16755 -0.00033 -0.00169 -0.00025 -0.00194 2.16561

A41 2.22694 0.00007 0.00054 0.00064 0.00117 2.22811

A42 1.91079 -0.00006 0.00004 0.00008 0.00011 1.91090

A43 2.19563 0.00033 0.00077 0.00113 0.00190 2.19753

A44 2.17677 -0.00026 -0.00081 -0.00121 -0.00202 2.17476

A45 2.16786 0.00023 0.00207 -0.00060 0.00147 2.16933

A46 2.22855 -0.00023 -0.00111 0.00027 -0.00084 2.22771

A47 1.88678 0.00000 -0.00096 0.00033 -0.00063 1.88615

A48 2.15048 0.00009 -0.00134 -0.00083 -0.00218 2.14829

A49 1.91256 -0.00000 0.00020 -0.00028 -0.00009 1.91247

A50 2.18562 0.00038 0.00071 0.00137 0.00209 2.18771

A51 2.18501 -0.00038 -0.00091 -0.00109 -0.00200 2.18301

A52 2.24387 -0.00051 0.00055 -0.00107 -0.00052 2.24334

A53 2.14979 0.00006 -0.00169 0.00084 -0.00085 2.14894

A54 1.88953 0.00045 0.00114 0.00023 0.00137 1.89090

A55 1.85735 -0.00058 -0.00181 -0.00017 -0.00199 1.85537

A56 2.15921 0.00032 -0.00034 0.00042 0.00008 2.15929

A57 2.26663 0.00026 0.00215 -0.00025 0.00190 2.26853

A58 1.88112 0.00011 0.00156 -0.00037 0.00120 1.88232

A59 2.22650 -0.00003 -0.00041 0.00016 -0.00025 2.22625

A60 2.17557 -0.00009 -0.00116 0.00021 -0.00095 2.17462

A61 1.88422 0.00002 -0.00109 0.00060 -0.00049 1.88373

A62 2.21052 -0.00057 -0.00170 -0.00111 -0.00280 2.20772

A63 2.18844 0.00056 0.00279 0.00051 0.00329 2.19174

A64 2.18777 0.00109 0.00330 0.00189 0.00520 2.19297

A65 1.56385 -0.00036 -0.00123 -0.00124 -0.00246 1.56139

A66 1.57775 0.00036 0.00123 0.00124 0.00246 1.58021

A67 1.57775 0.00036 0.00123 0.00124 0.00246 1.58021

A68 1.56385 -0.00036 -0.00123 -0.00124 -0.00246 1.56139

A69 1.94538 0.00002 0.00050 0.00005 0.00055 1.94593

A70 1.93825 -0.00012 0.00004 -0.00071 -0.00066 1.93758

A71 1.93825 -0.00012 0.00004 -0.00071 -0.00066 1.93758

A72 1.89253 0.00001 -0.00001 -0.00009 -0.00009 1.89244

A73 1.89253 0.00001 -0.00001 -0.00009 -0.00009 1.89244

A74 1.85372 0.00020 -0.00062 0.00162 0.00100 1.85472

A75 1.93763 -0.00007 0.00028 -0.00057 -0.00028 1.93735

A76 1.93763 -0.00007 0.00028 -0.00057 -0.00028 1.93735

A77 1.94344 -0.00003 -0.00032 0.00027 -0.00006 1.94339

A78 1.85715 0.00017 -0.00019 0.00135 0.00115 1.85831

A79 1.89253 0.00000 -0.00003 -0.00021 -0.00024 1.89229

A80 1.89253 0.00000 -0.00003 -0.00021 -0.00024 1.89229

A81 1.93763 -0.00007 0.00028 -0.00057 -0.00028 1.93735

A82 1.93763 -0.00007 0.00028 -0.00057 -0.00028 1.93735

A83 1.94344 -0.00003 -0.00032 0.00027 -0.00006 1.94339

A84 1.85715 0.00017 -0.00019 0.00135 0.00115 1.85831

A85 1.89253 0.00000 -0.00003 -0.00021 -0.00024 1.89229

A86 1.89253 0.00000 -0.00003 -0.00021 -0.00024 1.89229

A87 1.93825 -0.00012 0.00004 -0.00071 -0.00066 1.93758

A88 1.93825 -0.00012 0.00004 -0.00071 -0.00066 1.93758

A89 1.94538 0.00002 0.00050 0.00005 0.00055 1.94593

A90 1.85372 0.00020 -0.00062 0.00162 0.00100 1.85472

A91 1.89253 0.00001 -0.00001 -0.00009 -0.00009 1.89244

A92 1.89253 0.00001 -0.00001 -0.00009 -0.00009 1.89244

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

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D16 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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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

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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

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D29 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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D34 2.11228 -0.00005 0.00036 -0.00056 -0.00020 2.11208

D35 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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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

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D67 2.11054 -0.00006 -0.00006 -0.00048 -0.00054 2.11000

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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

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D74 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D78 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D79 -2.11054 0.00006 0.00006 0.00048 0.00054 -2.11000

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D83 -1.03106 -0.00006 -0.00006 -0.00048 -0.00054 -1.03160

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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

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D112 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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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 1.02931 0.00005 -0.00036 0.00056 0.00020 1.02951

D126 -1.02931 -0.00005 0.00036 -0.00056 -0.00020 -1.02951

D127 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D128 -2.11228 0.00005 -0.00036 0.00056 0.00020 -2.11208

D129 2.11228 -0.00005 0.00036 -0.00056 -0.00020 2.11208

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 0.001797 0.000450 NO

RMS Force 0.000367 0.000300 NO

Maximum Displacement 0.006450 0.001800 NO

RMS Displacement 0.001487 0.001200 NO

Predicted change in Energy=-5.728535D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 13:54:52 2019, MaxMem= 2415919104 cpu: 1.3

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.085110 -2.190241 0.000000

2 7 0 -0.737541 -1.866355 0.000000

3 6 0 -0.005013 -2.990440 0.000000

4 6 0 -0.934744 -4.156404 0.000000

5 6 0 -2.197018 -3.639635 0.000000

6 7 0 1.339364 -3.118545 0.000000

7 6 0 2.179516 -2.063516 0.000000

8 7 0 1.857806 -0.754451 0.000000

9 6 0 3.011220 0.003019 0.000000

10 6 0 4.166998 -0.920874 0.000000

11 6 0 3.649560 -2.177946 0.000000

12 7 0 -3.111944 -1.328862 0.000000

13 6 0 -4.166998 0.920874 0.000000

14 6 0 -3.649560 2.177946 0.000000

15 6 0 -2.179516 2.063516 0.000000

16 7 0 -1.857806 0.754451 0.000000

17 6 0 -3.011220 -0.003019 0.000000

18 7 0 -1.339364 3.118545 0.000000

19 7 0 0.737541 1.866355 0.000000

20 6 0 0.005013 2.990440 0.000000

21 6 0 0.934744 4.156404 0.000000

22 6 0 2.197018 3.639635 0.000000

23 6 0 2.085110 2.190241 0.000000

24 7 0 3.111944 1.328862 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.482602 -5.572024 0.000000

27 1 0 -3.131651 -4.183197 0.000000

28 6 0 5.588233 -0.481150 0.000000

29 1 0 4.188833 -3.114948 0.000000

30 6 0 -5.588233 0.481150 0.000000

31 1 0 -4.188833 3.114948 0.000000

32 6 0 0.482602 5.572024 0.000000

33 1 0 3.131651 4.183197 0.000000

34 1 0 -1.328120 -6.261779 0.000000

35 1 0 0.138663 -5.785890 0.876179

36 1 0 0.138663 -5.785890 -0.876179

37 1 0 5.807906 0.135994 0.876823

38 1 0 5.807906 0.135994 -0.876823

39 1 0 6.267970 -1.334478 0.000000

40 1 0 -5.807906 -0.135994 0.876823

41 1 0 -5.807906 -0.135994 -0.876823

42 1 0 -6.267970 1.334478 0.000000

43 1 0 -0.138663 5.785890 0.876179

44 1 0 -0.138663 5.785890 -0.876179

45 1 0 1.328120 6.261779 0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.385946 0.000000

3 C 2.228704 1.341702 0.000000

4 C 2.277968 2.298525 1.491266 0.000000

5 C 1.453708 2.296649 2.286119 1.363959 0.000000

6 N 3.548066 2.425183 1.350467 2.499744 3.574567

7 C 4.266509 2.923713 2.373048 3.752172 4.651688

8 N 4.196198 2.823501 2.910282 4.401320 4.976533

9 C 5.548240 4.189005 4.249524 5.733361 6.355680

10 C 6.379666 4.994840 4.657121 6.041227 6.920430

11 C 5.734683 4.398152 3.743801 4.993009 6.026525

12 N 1.340284 2.434479 3.523331 3.568640 2.485309

13 C 3.743433 4.419255 5.711435 6.018822 4.967803

14 C 4.639888 4.983595 6.324155 6.891604 5.996176

15 C 4.254804 4.186069 5.501903 6.343253 5.703178

16 N 2.953452 2.850196 4.178163 4.996853 4.407160

17 C 2.375209 2.939666 4.238156 4.643529 3.726648

18 N 5.360908 5.021097 6.253014 7.286192 6.812383

19 N 4.941996 4.013600 4.913231 6.250613 6.239195

20 C 5.586418 4.913231 5.980888 7.208364 6.986188

21 C 7.028472 6.250613 7.208364 8.520432 8.401557

22 C 7.233538 6.239195 6.986188 8.401557 8.502666

23 C 6.048087 4.941996 5.586418 7.028472 7.233538

24 N 6.276421 5.002793 5.326517 6.816438 7.271247

25 Zn 3.024043 2.006800 2.990444 4.260216 4.251333

26 C 3.742257 3.714429 2.625389 1.486073 2.583283

27 H 2.251027 3.331595 3.346422 2.197071 1.081203

28 C 7.861373 6.475663 6.130329 7.487104 8.401557

29 H 6.341723 5.082140 4.195694 5.228353 6.407370

30 C 4.405474 5.388877 6.574518 6.569769 5.336779

31 H 5.707072 6.060098 7.401359 7.966282 7.042139

32 C 8.175934 7.537786 8.576337 9.831133 9.593489

33 H 8.236219 7.181067 7.829414 9.278174 9.465274

34 H 4.141311 4.434923 3.528778 2.141810 2.762358

35 H 4.317587 4.110740 2.933066 2.138953 3.290822

36 H 4.317587 4.110740 2.933066 2.138953 3.290822

37 H 8.275258 6.900804 6.658335 8.040947 8.893987

38 H 8.275258 6.900804 6.658335 8.040947 8.893987

39 H 8.396802 7.025673 6.487875 7.735784 8.773242

40 H 4.341424 5.428772 6.526120 6.378105 5.107136

41 H 4.341424 5.428772 6.526120 6.378105 5.107136

42 H 5.469914 6.389912 7.611146 7.654612 6.427632

43 H 8.256816 7.725490 8.820971 10.012525 9.687365

44 H 8.256816 7.725490 8.820971 10.012525 9.687365

45 H 9.115195 8.386508 9.347769 10.661102 10.510214

6 7 8 9 10

6 N 0.000000

7 C 1.348681 0.000000

8 N 2.420273 1.348016 0.000000

9 C 3.541082 2.227621 1.379900 0.000000

10 C 3.581238 2.292534 2.315181 1.479663 0.000000

11 C 2.494340 1.474491 2.288388 2.272462 1.359401

12 N 4.797615 5.342216 5.002836 6.266342 7.290367

13 C 6.829123 7.013189 6.253397 7.236661 8.535075

14 C 7.276137 7.208892 6.239394 7.006875 8.408404

15 C 6.263886 6.002796 4.923506 5.584746 7.013189

16 N 5.022150 4.923506 4.010307 4.926668 6.253397

17 C 5.351082 5.584746 4.926668 6.022442 7.236661

18 N 6.787994 6.263886 5.022150 5.351082 6.829123

19 N 5.021097 4.186069 2.850196 2.939666 4.419255

20 C 6.253014 5.501903 4.178163 4.238156 5.711435

21 C 7.286192 6.343253 4.996853 4.643529 6.018822

22 C 6.812383 5.703178 4.407160 3.726648 4.967803

23 C 5.360908 4.254804 2.953452 2.375209 3.743433

24 N 4.787637 3.518188 2.431677 1.329664 2.484844

25 Zn 3.393997 3.001398 2.005153 3.011221 4.267538

26 C 3.055997 4.404146 5.355980 6.579353 6.576623

27 H 4.596027 5.718527 6.054006 7.433658 7.994562

28 C 5.000874 3.758089 3.740425 2.622102 1.487706

29 H 2.849472 2.267788 3.317474 3.332940 2.194182

30 C 7.807010 8.173938 7.547861 8.612734 9.855465

31 H 8.331710 8.208067 7.178725 7.843779 9.279427

32 C 8.732699 7.821828 6.474216 6.116186 7.465420

33 H 7.518493 6.318860 5.099319 4.181913 5.208022

34 H 4.122547 5.470733 6.362451 7.620863 7.663001

35 H 3.053540 4.334610 5.388741 6.521560 6.376798

36 H 3.053540 4.334610 5.388741 6.521560 6.376798

37 H 5.597205 4.332652 4.143066 2.933932 2.139712

38 H 5.597205 4.332652 4.143066 2.933932 2.139712

39 H 5.241570 4.152945 4.448143 3.520699 2.141297

40 H 7.794094 8.263357 7.740443 8.863697 10.044081

41 H 7.794094 8.263357 7.740443 8.863697 10.044081

42 H 8.814814 9.105294 8.389986 9.374228 10.675915

43 H 9.068694 8.231332 6.894175 6.643121 8.017923

44 H 9.068694 8.231332 6.894175 6.643121 8.017923

45 H 9.380330 8.368716 7.036196 6.481119 7.723324

11 12 13 14 15

11 C 0.000000

12 N 6.814608 0.000000

13 C 8.408404 2.484844 0.000000

14 C 8.500055 3.547778 1.359401 0.000000

15 C 7.208892 3.518188 2.292534 1.474491 0.000000

16 N 6.239394 2.431677 2.315181 2.288388 1.348016

17 C 7.006875 1.329664 1.479663 2.272462 2.227621

18 N 7.276137 4.787637 3.581238 2.494340 1.348681

19 N 4.983595 5.002793 4.994840 4.398152 2.923713

20 C 6.324155 5.326517 4.657121 3.743801 2.373048

21 C 6.891604 6.816438 6.041227 4.993009 3.752172

22 C 5.996176 7.271247 6.920430 6.026525 4.651688

23 C 4.639888 6.276421 6.379666 5.734683 4.266509

24 N 3.547778 6.767590 7.290367 6.814608 5.342216

25 Zn 4.250028 3.383795 4.267538 4.250028 3.001398

26 C 5.347385 4.991780 7.465420 8.372076 7.821828

27 H 7.071482 2.854403 5.208022 6.382192 6.318860

28 C 2.576348 8.741379 9.855465 9.612888 8.173938

29 H 1.081105 7.516080 9.279427 9.458072 8.208067

30 C 9.612888 3.067271 1.487706 2.576348 3.758089

31 H 9.458072 4.572432 2.194182 1.081105 2.267788

32 C 8.372076 7.780937 6.576623 5.347385 4.404146

33 H 6.382192 8.328582 7.994562 7.071482 5.718527

34 H 6.438555 5.245541 7.723324 8.753173 8.368716

35 H 5.109927 5.585628 8.017923 8.862337 8.231332

36 H 5.109927 5.585628 8.017923 8.862337 8.231332

37 H 3.283533 9.081759 10.044081 9.715042 8.263357

38 H 3.283533 9.081759 10.044081 9.715042 8.263357

39 H 2.750911 9.379916 10.675915 10.521146 9.105294

40 H 9.715042 3.075705 2.139712 3.283533 4.332652

41 H 9.715042 3.075705 2.139712 3.283533 4.332652

42 H 10.521146 4.129634 2.141297 2.750911 4.152945

43 H 8.862337 7.760657 6.376798 5.109927 4.334610

44 H 8.862337 7.760657 6.376798 5.109927 4.334610

45 H 8.753173 8.793861 7.663001 6.438555 5.470733

16 17 18 19 20

16 N 0.000000

17 C 1.379900 0.000000

18 N 2.420273 3.541082 0.000000

19 N 2.823501 4.189005 2.425183 0.000000

20 C 2.910282 4.249524 1.350467 1.341702 0.000000

21 C 4.401320 5.733361 2.499744 2.298525 1.491266

22 C 4.976533 6.355680 3.574567 2.296649 2.286119

23 C 4.196198 5.548240 3.548066 1.385946 2.228704

24 N 5.002836 6.266342 4.797615 2.434479 3.523331

25 Zn 2.005153 3.011221 3.393997 2.006800 2.990444

26 C 6.474216 6.116186 8.732699 7.537786 8.576337

27 H 5.099319 4.181913 7.518493 7.181067 7.829414

28 C 7.547861 8.612734 7.807010 5.388877 6.574518

29 H 7.178725 7.843779 8.331710 6.060098 7.401359

30 C 3.740425 2.622102 5.000874 6.475663 6.130329

31 H 3.317474 3.332940 2.849472 5.082140 4.195694

32 C 5.355980 6.579353 3.055997 3.714429 2.625389

33 H 6.054006 7.433658 4.596027 3.331595 3.346422

34 H 7.036196 6.481119 9.380330 8.386508 9.347769

35 H 6.894175 6.643121 9.068694 7.725490 8.820971

36 H 6.894175 6.643121 9.068694 7.725490 8.820971

37 H 7.740443 8.863697 7.794094 5.428772 6.526120

38 H 7.740443 8.863697 7.794094 5.428772 6.526120

39 H 8.389986 9.374228 8.814814 6.389912 7.611146

40 H 4.143066 2.933932 5.597205 6.900804 6.658335

41 H 4.143066 2.933932 5.597205 6.900804 6.658335

42 H 4.448143 3.520699 5.241570 7.025673 6.487875

43 H 5.388741 6.521560 3.053540 4.110740 2.933066

44 H 5.388741 6.521560 3.053540 4.110740 2.933066

45 H 6.362451 7.620863 4.122547 4.434923 3.528778

21 22 23 24 25

21 C 0.000000

22 C 1.363959 0.000000

23 C 2.277968 1.453708 0.000000

24 N 3.568640 2.485309 1.340284 0.000000

25 Zn 4.260216 4.251333 3.024043 3.383795 0.000000

26 C 9.831133 9.593489 8.175934 7.780937 5.592884

27 H 9.278174 9.465274 8.236219 8.328582 5.225551

28 C 6.569769 5.336779 4.405474 3.067271 5.608909

29 H 7.966282 7.042139 5.707072 4.572432 5.220079

30 C 7.487104 8.401557 7.861373 8.741379 5.608909

31 H 5.228353 6.407370 6.341723 7.516080 5.220079

32 C 1.486073 2.583283 3.742257 4.991780 5.592884

33 H 2.197071 1.081203 2.251027 2.854403 5.225551

34 H 10.661102 10.510214 9.115195 8.793861 6.401076

35 H 10.012525 9.687365 8.256816 7.760657 5.853499

36 H 10.012525 9.687365 8.256816 7.760657 5.853499

37 H 6.378105 5.107136 4.341424 3.075705 5.875294

38 H 6.378105 5.107136 4.341424 3.075705 5.875294

39 H 7.654612 6.427632 5.469914 4.129634 6.408454

40 H 8.040947 8.893987 8.275258 9.081759 5.875294

41 H 8.040947 8.893987 8.275258 9.081759 5.875294

42 H 7.735784 8.773242 8.396802 9.379916 6.408454

43 H 2.138953 3.290822 4.317587 5.585628 5.853499

44 H 2.138953 3.290822 4.317587 5.585628 5.853499

45 H 2.141810 2.762358 4.141311 5.245541 6.401076

26 27 28 29 30

26 C 0.000000

27 H 2.991037 0.000000

28 C 7.922880 9.473201 0.000000

29 H 5.278213 7.398017 2.982484 0.000000

30 C 7.918863 5.271710 11.217817 10.417435 0.000000

31 H 9.444556 7.374317 10.417435 10.440158 2.982484

32 C 11.185769 10.403229 7.918863 9.444556 7.922880

33 H 10.403229 10.451101 5.271710 7.374317 9.473201

34 H 1.091175 2.751950 9.013968 6.351324 7.975942

35 H 1.095171 3.745834 7.655441 4.930061 8.534684

36 H 1.095171 3.745834 7.655441 4.930061 8.534684

37 H 8.539366 9.966941 1.094505 3.736153 11.435031

38 H 8.539366 9.966941 1.094505 3.736153 11.435031

39 H 7.970384 9.821817 1.090968 2.737313 11.994418

40 H 7.660164 4.930620 11.435031 10.467941 1.094505

41 H 7.660164 4.930620 11.435031 10.467941 1.094505

42 H 9.009453 6.346750 11.994418 11.364072 1.090968

43 H 11.396851 10.445496 8.534684 9.935786 7.655441

44 H 11.396851 10.445496 8.534684 9.935786 7.655441

45 H 11.971533 11.357248 7.975942 9.803402 9.013968

31 32 33 34 35

31 H 0.000000

32 C 5.278213 0.000000

33 H 7.398017 2.991037 0.000000

34 H 9.803402 11.971533 11.357248 0.000000

35 H 9.935786 11.396851 10.445496 1.773587 0.000000

36 H 9.935786 11.396851 10.445496 1.773587 1.752359

37 H 10.467941 7.660164 4.930620 9.624094 8.198111

38 H 10.467941 7.660164 4.930620 9.624094 8.383439

39 H 11.364072 9.009453 6.346750 9.054219 7.625692

40 H 3.736153 8.539366 9.966941 7.639538 8.202622

41 H 3.736153 8.539366 9.966941 7.639538 8.387850

42 H 2.737313 7.970384 9.821817 9.061194 9.618330

43 H 4.930061 1.095171 3.745834 12.137909 11.575104

44 H 4.930061 1.095171 3.745834 12.137909 11.706997

45 H 6.351324 1.091175 2.751950 12.802153 12.137909

36 37 38 39 40

36 H 0.000000

37 H 8.383439 0.000000

38 H 8.198111 1.753646 0.000000

39 H 7.625692 1.772784 1.772784 0.000000

40 H 8.387850 11.618996 11.750589 12.166839 0.000000

41 H 8.202622 11.750589 11.618996 12.166839 1.753646

42 H 9.618330 12.166839 12.166839 12.816907 1.772784

43 H 11.706997 8.202622 8.387850 9.618330 8.198111

44 H 11.575104 8.387850 8.202622 9.618330 8.383439

45 H 12.137909 7.639538 7.639538 9.061194 9.624094

41 42 43 44 45

41 H 0.000000

42 H 1.772784 0.000000

43 H 8.383439 7.625692 0.000000

44 H 8.198111 7.625692 1.752359 0.000000

45 H 9.624094 9.054219 1.773587 1.773587 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=3 Diff= 1.94D-03

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 -2.813828 1.107796 0.000000

2 7 0 -2.006711 -0.018884 0.000000

3 6 0 -2.772575 -1.120526 0.000000

4 6 0 -4.202677 -0.697817 0.000000

5 6 0 -4.198820 0.666137 0.000000

6 7 0 -2.385437 -2.414313 0.000000

7 6 0 -1.091824 -2.795767 0.000000

8 7 0 0.000000 -2.005153 0.000000

9 6 0 1.135786 -2.788806 0.000000

10 6 0 0.714653 -4.207273 0.000000

11 6 0 -0.644732 -4.200840 0.000000

12 7 0 -2.402099 2.383273 0.000000

13 6 0 -0.714653 4.207273 0.000000

14 6 0 0.644732 4.200840 0.000000

15 6 0 1.091824 2.795767 0.000000

16 7 0 0.000000 2.005153 0.000000

17 6 0 -1.135786 2.788806 0.000000

18 7 0 2.385437 2.414313 0.000000

19 7 0 2.006711 0.018884 0.000000

20 6 0 2.772575 1.120526 0.000000

21 6 0 4.202677 0.697817 0.000000

22 6 0 4.198820 -0.666137 0.000000

23 6 0 2.813828 -1.107796 0.000000

24 7 0 2.402099 -2.383273 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -5.344150 -1.649370 0.000000

27 1 0 -5.054101 1.327571 0.000000

28 6 0 1.656814 -5.358621 0.000000

29 1 0 -1.309974 -5.053038 0.000000

30 6 0 -1.656814 5.358621 0.000000

31 1 0 1.309974 5.053038 0.000000

32 6 0 5.344150 1.649370 0.000000

33 1 0 5.054101 -1.327571 0.000000

34 1 0 -6.301350 -1.125508 0.000000

35 1 0 -5.308546 -2.305450 0.876179

36 1 0 -5.308546 -2.305450 -0.876179

37 1 0 2.311260 -5.329948 0.876823

38 1 0 2.311260 -5.329948 -0.876823

39 1 0 1.121947 -6.309478 0.000000

40 1 0 -2.311260 5.329948 0.876823

41 1 0 -2.311260 5.329948 -0.876823

42 1 0 -1.121947 6.309478 0.000000

43 1 0 5.308546 2.305450 0.876179

44 1 0 5.308546 2.305450 -0.876179

45 1 0 6.301350 1.125508 0.000000

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

Rotational constants (GHZ): 0.1829156 0.1819082 0.0914096

Leave Link 202 at Tue Sep 17 13:54:52 2019, MaxMem= 2415919104 cpu: 0.1

(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 101 beta electrons

nuclear repulsion energy 2761.5759910063 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= -0.1142495563 Hartrees.

Nuclear repulsion after empirical dispersion term = 2761.4617414500 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 = 3488

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.25D-08

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 128

GePol: Fraction of low-weight points (<1% of avg) = 3.67%

GePol: Cavity surface area = 382.154 Ang\*\*2

GePol: Cavity volume = 379.438 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0107279588 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2761.4510134912 Hartrees.

Leave Link 301 at Tue Sep 17 13:54:52 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= 15327 LenP2D= 41276.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.85D-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 13:54:53 2019, MaxMem= 2415919104 cpu: 11.8

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 13:54:53 2019, MaxMem= 2415919104 cpu: 1.6

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= 0.000000 0.000000 -0.000000

Rot= 1.000000 0.000000 -0.000000 -0.000655 Ang= -0.08 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 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0426 S= 1.0141

Leave Link 401 at Tue Sep 17 13:54:54 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= 36498432.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.66D-15 for 3473.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.04D-15 for 2269 2135.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.22D-15 for 3473.

Iteration 1 A^-1\*A deviation from orthogonality is 6.24D-13 for 2148 1154.

E= -1275.84063935955

DIIS: error= 2.36D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.84063935955 IErMin= 1 ErrMin= 2.36D-04

ErrMax= 2.36D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.86D-04 BMatP= 1.86D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.36D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.299 Goal= None Shift= 0.000

Gap= 0.396 Goal= None Shift= 0.000

RMSDP=2.31D-05 MaxDP=5.65D-04 OVMax= 1.12D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.31D-05 CP: 1.00D+00

E= -1275.84071187001 Delta-E= -0.000072510458 Rises=F Damp=F

DIIS: error= 1.39D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84071187001 IErMin= 2 ErrMin= 1.39D-04

ErrMax= 1.39D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.63D-05 BMatP= 1.86D-04

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.39D-03

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

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

Coeff: 0.141D+00 0.859D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=1.14D-05 MaxDP=4.82D-04 DE=-7.25D-05 OVMax= 6.79D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.02D-05 CP: 1.00D+00 1.22D+00

E= -1275.84071570748 Delta-E= -0.000003837467 Rises=F Damp=F

DIIS: error= 2.60D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1275.84071570748 IErMin= 2 ErrMin= 1.39D-04

ErrMax= 2.60D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.79D-05 BMatP= 2.63D-05

IDIUse=3 WtCom= 3.83D-01 WtEn= 6.17D-01

Coeff-Com: -0.110D-01 0.554D+00 0.457D+00

Coeff-En: 0.000D+00 0.357D+00 0.643D+00

Coeff: -0.420D-02 0.432D+00 0.572D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=9.56D-06 MaxDP=3.84D-04 DE=-3.84D-06 OVMax= 5.00D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 8.18D-06 CP: 1.00D+00 1.41D+00 7.91D-01

E= -1275.84072528378 Delta-E= -0.000009576300 Rises=F Damp=F

DIIS: error= 1.37D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84072528378 IErMin= 4 ErrMin= 1.37D-04

ErrMax= 1.37D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.36D-05 BMatP= 2.63D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.37D-03

Coeff-Com: -0.101D-01 0.867D-01 0.381D+00 0.543D+00

Coeff-En: 0.000D+00 0.000D+00 0.137D+00 0.863D+00

Coeff: -0.100D-01 0.865D-01 0.380D+00 0.543D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=5.80D-06 MaxDP=2.13D-04 DE=-9.58D-06 OVMax= 3.99D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.84D-06 CP: 1.00D+00 1.53D+00 1.26D+00 1.11D+00

E= -1275.84073099298 Delta-E= -0.000005709198 Rises=F Damp=F

DIIS: error= 9.63D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84073099298 IErMin= 5 ErrMin= 9.63D-05

ErrMax= 9.63D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.02D-06 BMatP= 1.36D-05

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

Coeff-Com: 0.179D-02-0.124D+00 0.878D-01 0.279D+00 0.756D+00

Coeff: 0.179D-02-0.124D+00 0.878D-01 0.279D+00 0.756D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=6.58D-06 MaxDP=2.71D-04 DE=-5.71D-06 OVMax= 5.28D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 8.88D-07 CP: 1.00D+00 1.70D+00 1.60D+00 1.57D+00 1.37D+00

E= -1275.84073410657 Delta-E= -0.000003113589 Rises=F Damp=F

DIIS: error= 7.72D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84073410657 IErMin= 6 ErrMin= 7.72D-05

ErrMax= 7.72D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.01D-07 BMatP= 1.02D-06

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

Coeff-Com: 0.124D-01-0.184D+00-0.268D+00-0.309D+00 0.264D+00 0.148D+01

Coeff: 0.124D-01-0.184D+00-0.268D+00-0.309D+00 0.264D+00 0.148D+01

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=1.38D-05 MaxDP=5.66D-04 DE=-3.11D-06 OVMax= 1.11D-02

Cycle 7 Pass 1 IDiag 1:

RMSU= 8.70D-07 CP: 1.00D+00 2.04D+00 2.37D+00 2.50D+00 2.74D+00

CP: 2.34D+00

E= -1275.84073820474 Delta-E= -0.000004098172 Rises=F Damp=F

DIIS: error= 3.65D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84073820474 IErMin= 7 ErrMin= 3.65D-05

ErrMax= 3.65D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.02D-07 BMatP= 5.01D-07

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

Coeff-Com: 0.882D-02-0.899D-01-0.233D+00-0.349D+00-0.131D+00 0.112D+01

Coeff-Com: 0.675D+00

Coeff: 0.882D-02-0.899D-01-0.233D+00-0.349D+00-0.131D+00 0.112D+01

Coeff: 0.675D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=7.53D-06 MaxDP=3.08D-04 DE=-4.10D-06 OVMax= 6.07D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.06D-06 CP: 1.00D+00 2.23D+00 2.78D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.30D+00

E= -1275.84073922639 Delta-E= -0.000001021649 Rises=F Damp=F

DIIS: error= 1.36D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84073922639 IErMin= 8 ErrMin= 1.36D-05

ErrMax= 1.36D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.20D-08 BMatP= 3.02D-07

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

Coeff-Com: -0.179D-02 0.468D-01 0.480D-01 0.233D-01-0.129D+00-0.235D+00

Coeff-Com: 0.242D+00 0.101D+01

Coeff: -0.179D-02 0.468D-01 0.480D-01 0.233D-01-0.129D+00-0.235D+00

Coeff: 0.242D+00 0.101D+01

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=2.60D-06 MaxDP=1.06D-04 DE=-1.02D-06 OVMax= 2.07D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.42D-06 CP: 1.00D+00 2.29D+00 2.92D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.77D+00 1.79D+00

E= -1275.84073941404 Delta-E= -0.000000187651 Rises=F Damp=F

DIIS: error= 6.60D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84073941404 IErMin= 9 ErrMin= 6.60D-06

ErrMax= 6.60D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.70D-08 BMatP= 6.20D-08

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

Coeff-Com: -0.317D-02 0.448D-01 0.859D-01 0.103D+00-0.145D-01-0.422D+00

Coeff-Com: -0.760D-01 0.508D+00 0.774D+00

Coeff: -0.317D-02 0.448D-01 0.859D-01 0.103D+00-0.145D-01-0.422D+00

Coeff: -0.760D-01 0.508D+00 0.774D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=1.10D-06 MaxDP=4.45D-05 DE=-1.88D-07 OVMax= 8.58D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.81D-07 CP: 1.00D+00 2.31D+00 2.98D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.00D+00 2.21D+00 1.39D+00

E= -1275.84073946655 Delta-E= -0.000000052512 Rises=F Damp=F

DIIS: error= 4.10D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84073946655 IErMin=10 ErrMin= 4.10D-06

ErrMax= 4.10D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.95D-09 BMatP= 2.70D-08

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

Coeff-Com: -0.396D-03-0.509D-02 0.164D-01 0.406D-01 0.673D-01-0.906D-01

Coeff-Com: -0.164D+00-0.223D+00 0.309D+00 0.105D+01

Coeff: -0.396D-03-0.509D-02 0.164D-01 0.406D-01 0.673D-01-0.906D-01

Coeff: -0.164D+00-0.223D+00 0.309D+00 0.105D+01

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=7.96D-07 MaxDP=3.05D-05 DE=-5.25D-08 OVMax= 6.05D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 2.03D-07 CP: 1.00D+00 2.33D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.19D+00 2.50D+00 1.68D+00 1.56D+00

E= -1275.84073948893 Delta-E= -0.000000022384 Rises=F Damp=F

DIIS: error= 2.10D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84073948893 IErMin=11 ErrMin= 2.10D-06

ErrMax= 2.10D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.73D-09 BMatP= 7.95D-09

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

Coeff-Com: 0.639D-03-0.149D-01-0.165D-01-0.962D-02 0.281D-01 0.673D-01

Coeff-Com: -0.482D-01-0.195D+00-0.584D-01 0.502D+00 0.744D+00

Coeff: 0.639D-03-0.149D-01-0.165D-01-0.962D-02 0.281D-01 0.673D-01

Coeff: -0.482D-01-0.195D+00-0.584D-01 0.502D+00 0.744D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=4.15D-07 MaxDP=1.68D-05 DE=-2.24D-08 OVMax= 3.29D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.58D-07 CP: 1.00D+00 2.34D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.25D+00 2.62D+00 1.84D+00 1.84D+00

CP: 1.78D+00

E= -1275.84073949381 Delta-E= -0.000000004877 Rises=F Damp=F

DIIS: error= 1.26D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84073949381 IErMin=12 ErrMin= 1.26D-06

ErrMax= 1.26D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.02D-09 BMatP= 2.73D-09

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

Coeff-Com: 0.528D-03-0.717D-02-0.150D-01-0.187D-01-0.829D-02 0.734D-01

Coeff-Com: 0.270D-01-0.409D-01-0.161D+00-0.786D-01 0.465D+00 0.764D+00

Coeff: 0.528D-03-0.717D-02-0.150D-01-0.187D-01-0.829D-02 0.734D-01

Coeff: 0.270D-01-0.409D-01-0.161D+00-0.786D-01 0.465D+00 0.764D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=2.17D-07 MaxDP=8.22D-06 DE=-4.88D-09 OVMax= 1.68D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 3.25D-08 CP: 1.00D+00 2.35D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.28D+00 2.68D+00 1.92D+00 2.03D+00

CP: 2.26D+00 1.35D+00

E= -1275.84073949526 Delta-E= -0.000000001448 Rises=F Damp=F

DIIS: error= 4.15D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84073949526 IErMin=13 ErrMin= 4.15D-07

ErrMax= 4.15D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.11D-10 BMatP= 1.02D-09

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

Coeff-Com: -0.214D-04 0.197D-02 0.979D-03-0.175D-02-0.101D-01 0.158D-02

Coeff-Com: 0.170D-01 0.365D-01-0.235D-01-0.152D+00-0.621D-01 0.205D+00

Coeff-Com: 0.987D+00

Coeff: -0.214D-04 0.197D-02 0.979D-03-0.175D-02-0.101D-01 0.158D-02

Coeff: 0.170D-01 0.365D-01-0.235D-01-0.152D+00-0.621D-01 0.205D+00

Coeff: 0.987D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=9.51D-08 MaxDP=3.77D-06 DE=-1.45D-09 OVMax= 7.27D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 1.34D-08 CP: 1.00D+00 2.35D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.30D+00 2.71D+00 1.96D+00 2.11D+00

CP: 2.48D+00 1.52D+00 1.10D+00

E= -1275.84073949551 Delta-E= -0.000000000252 Rises=F Damp=F

DIIS: error= 1.62D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84073949551 IErMin=14 ErrMin= 1.62D-07

ErrMax= 1.62D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.70D-11 BMatP= 1.11D-10

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

Coeff-Com: -0.672D-04 0.185D-02 0.192D-02 0.461D-03-0.530D-02-0.668D-02

Coeff-Com: 0.734D-02 0.264D-01 0.524D-02-0.817D-01-0.821D-01 0.167D-01

Coeff-Com: 0.528D+00 0.588D+00

Coeff: -0.672D-04 0.185D-02 0.192D-02 0.461D-03-0.530D-02-0.668D-02

Coeff: 0.734D-02 0.264D-01 0.524D-02-0.817D-01-0.821D-01 0.167D-01

Coeff: 0.528D+00 0.588D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=4.16D-08 MaxDP=1.61D-06 DE=-2.52D-10 OVMax= 3.30D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 5.13D-09 CP: 1.00D+00 2.35D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.30D+00 2.73D+00 1.97D+00 2.12D+00

CP: 2.57D+00 1.62D+00 1.25D+00 9.43D-01

E= -1275.84073949551 Delta-E= 0.000000000000 Rises=F Damp=F

DIIS: error= 8.93D-08 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=14 EnMin= -1275.84073949551 IErMin=15 ErrMin= 8.93D-08

ErrMax= 8.93D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.39D-12 BMatP= 3.70D-11

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

Coeff-Com: -0.247D-04 0.272D-03 0.798D-03 0.104D-02 0.107D-02-0.390D-02

Coeff-Com: -0.241D-02 0.548D-03 0.938D-02 0.510D-02-0.115D-01-0.562D-01

Coeff-Com: -0.272D-01 0.261D+00 0.822D+00

Coeff: -0.247D-04 0.272D-03 0.798D-03 0.104D-02 0.107D-02-0.390D-02

Coeff: -0.241D-02 0.548D-03 0.938D-02 0.510D-02-0.115D-01-0.562D-01

Coeff: -0.272D-01 0.261D+00 0.822D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=5.81D-09 MaxDP=3.78D-07 DE= 4.55D-13 OVMax= 3.53D-06

Error on total polarization charges = 0.06467

SCF Done: E(UB3LYP) = -1275.84073950 A.U. after 15 cycles

NFock= 15 Conv=0.58D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0419 S= 1.0139

<L.S>= 0.000000000000E+00

KE= 1.320801456383D+03 PE=-8.574843297463D+03 EE= 3.216750088093D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.73

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0419, after 2.0010

Leave Link 502 at Tue Sep 17 13:56:18 2019, MaxMem= 2415919104 cpu: 1481.5

(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= 15327 LenP2D= 41276.

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 = 245

Leave Link 701 at Tue Sep 17 13:56:22 2019, MaxMem= 2415919104 cpu: 71.2

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 13:56:22 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 13:56:35 2019, MaxMem= 2415919104 cpu: 232.4

(Enter /home/blab/g09/l716.exe)

Dipole =-5.86197757D-14 6.30606678D-14-6.66133815D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.001594709 -0.002442976 0.000000000

2 7 -0.000070985 0.000198113 0.000000000

3 6 -0.002693256 -0.001464346 -0.000000000

4 6 0.002032451 0.000518071 -0.000000000

5 6 -0.001032432 0.001560475 0.000000000

6 7 0.003088533 0.001958938 0.000000000

7 6 -0.001810794 -0.002213399 -0.000000000

8 7 -0.000093426 0.000490569 0.000000000

9 6 -0.000499217 0.002390786 -0.000000000

10 6 0.000291697 -0.001151672 -0.000000000

11 6 0.000942047 0.000486222 0.000000000

12 7 -0.001127063 0.003346844 0.000000000

13 6 -0.000291697 0.001151672 -0.000000000

14 6 -0.000942047 -0.000486222 0.000000000

15 6 0.001810794 0.002213399 -0.000000000

16 7 0.000093426 -0.000490569 -0.000000000

17 6 0.000499217 -0.002390786 0.000000000

18 7 -0.003088533 -0.001958938 -0.000000000

19 7 0.000070985 -0.000198113 0.000000000

20 6 0.002693256 0.001464346 0.000000000

21 6 -0.002032451 -0.000518071 -0.000000000

22 6 0.001032432 -0.001560475 -0.000000000

23 6 -0.001594709 0.002442976 -0.000000000

24 7 0.001127063 -0.003346844 0.000000000

25 30 0.000000000 -0.000000000 -0.000000000

26 6 -0.000016744 -0.000094513 0.000000000

27 1 0.000002200 -0.000064926 -0.000000000

28 6 0.000083467 0.000119539 0.000000000

29 1 -0.000004767 -0.000059863 -0.000000000

30 6 -0.000083467 -0.000119539 0.000000000

31 1 0.000004767 0.000059863 -0.000000000

32 6 0.000016744 0.000094513 0.000000000

33 1 -0.000002200 0.000064926 0.000000000

34 1 -0.000047350 -0.000036873 0.000000000

35 1 0.000001576 -0.000042008 0.000122175

36 1 0.000001576 -0.000042008 -0.000122175

37 1 -0.000048916 -0.000002230 0.000113552

38 1 -0.000048916 -0.000002230 -0.000113552

39 1 -0.000008940 -0.000063954 0.000000000

40 1 0.000048916 0.000002230 0.000113552

41 1 0.000048916 0.000002230 -0.000113552

42 1 0.000008940 0.000063954 0.000000000

43 1 -0.000001576 0.000042008 0.000122175

44 1 -0.000001576 0.000042008 -0.000122175

45 1 0.000047350 0.000036873 -0.000000000

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

Cartesian Forces: Max 0.003346844 RMS 0.001009141

Leave Link 716 at Tue Sep 17 13:56:35 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 0.002176841 RMS 0.000394492

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= -1.02D-04 DEPred=-5.73D-05 R= 1.78D+00

TightC=F SS= 1.41D+00 RLast= 2.37D-02 DXNew= 5.0454D-01 7.1165D-02

Trust test= 1.78D+00 RLast= 2.37D-02 DXMaxT set to 3.00D-01

ITU= 1 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01339

Eigenvalues --- 0.01341 0.01344 0.01345 0.01604 0.01622

Eigenvalues --- 0.01635 0.01636 0.01775 0.01791 0.01815

Eigenvalues --- 0.01816 0.01892 0.01908 0.01942 0.01947

Eigenvalues --- 0.01998 0.01999 0.02043 0.02049 0.02070

Eigenvalues --- 0.02088 0.02102 0.02112 0.02114 0.02205

Eigenvalues --- 0.02311 0.02318 0.02351 0.02373 0.05979

Eigenvalues --- 0.07177 0.07177 0.07203 0.07203 0.07338

Eigenvalues --- 0.07351 0.07353 0.07371 0.14491 0.14507

Eigenvalues --- 0.15952 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 0.16013 0.16058

Eigenvalues --- 0.16120 0.16710 0.18457 0.22067 0.22088

Eigenvalues --- 0.23841 0.23852 0.23881 0.24014 0.24715

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25088

Eigenvalues --- 0.25815 0.29952 0.32940 0.33194 0.33197

Eigenvalues --- 0.33282 0.33282 0.33296 0.33338 0.33710

Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33785 0.34388 0.34437 0.34437

Eigenvalues --- 0.34439 0.34891 0.35550 0.35564 0.35624

Eigenvalues --- 0.35682 0.35682 0.35745 0.37515 0.38555

Eigenvalues --- 0.40318 0.41707 0.41745 0.43015 0.47900

Eigenvalues --- 0.48938 0.49011 0.49542 0.51274 0.51345

Eigenvalues --- 0.51358 0.51361 0.54007 0.54038 0.54235

Eigenvalues --- 0.56304 0.56345 0.56380 0.91503

DIIS coeff's: 1.00455 0.50756 -0.70382 0.19171

Cosine: 0.879 > 0.710

Length: 0.660

GDIIS step was calculated using 4 of the last 4 vectors.

Iteration 1 RMS(Cart)= 0.00267921 RMS(Int)= 0.00000773

Iteration 2 RMS(Cart)= 0.00001329 RMS(Int)= 0.00000471

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000471

ITry= 1 IFail=0 DXMaxC= 1.30D-02 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 8.43D-10 for atom 38.

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

(Linear) (Quad) (Total)

R1 2.61906 -0.00039 0.00447 0.00240 0.00687 2.62593

R2 2.74711 -0.00097 -0.00156 -0.00728 -0.00884 2.73827

R3 2.53277 0.00197 0.00081 0.00338 0.00419 2.53696

R4 2.53545 0.00022 -0.00529 -0.00176 -0.00705 2.52840

R5 3.79230 0.00005 0.00295 -0.00015 0.00281 3.79511

R6 2.81808 -0.00117 0.00376 -0.00400 -0.00024 2.81784

R7 2.55201 0.00168 0.00287 0.00685 0.00972 2.56173

R8 2.57751 0.00125 0.00042 0.00567 0.00609 2.58360

R9 2.80827 0.00018 0.00004 -0.00086 -0.00082 2.80745

R10 2.04318 0.00003 0.00028 0.00093 0.00121 2.04438

R11 2.54864 -0.00218 0.00130 -0.00710 -0.00581 2.54283

R12 2.54738 0.00064 -0.00426 -0.00082 -0.00508 2.54230

R13 2.78638 0.00063 0.00324 0.00469 0.00792 2.79431

R14 2.60763 -0.00010 0.00336 0.00258 0.00593 2.61356

R15 3.78919 0.00006 0.00229 -0.00234 -0.00005 3.78914

R16 2.79616 0.00083 0.00154 0.00247 0.00402 2.80018

R17 2.51270 -0.00184 -0.00148 -0.00940 -0.01088 2.50182

R18 2.56889 -0.00059 -0.00101 -0.00145 -0.00246 2.56643

R19 2.81136 -0.00001 0.00035 0.00160 0.00195 2.81331

R20 2.04299 0.00005 0.00085 -0.00076 0.00009 2.04309

R21 2.51270 -0.00184 -0.00148 -0.00940 -0.01088 2.50182

R22 2.56889 -0.00059 -0.00101 -0.00145 -0.00246 2.56643

R23 2.79616 0.00083 0.00154 0.00247 0.00402 2.80018

R24 2.81136 -0.00001 0.00035 0.00160 0.00195 2.81331

R25 2.78638 0.00063 0.00324 0.00469 0.00792 2.79431

R26 2.04299 0.00005 0.00085 -0.00076 0.00009 2.04309

R27 2.54738 0.00064 -0.00426 -0.00082 -0.00508 2.54230

R28 2.54864 -0.00218 0.00130 -0.00710 -0.00581 2.54283

R29 2.60763 -0.00010 0.00336 0.00258 0.00593 2.61356

R30 3.78919 0.00006 0.00229 -0.00234 -0.00005 3.78914

R31 2.55201 0.00168 0.00287 0.00685 0.00972 2.56173

R32 2.53545 0.00022 -0.00529 -0.00176 -0.00705 2.52840

R33 2.61906 -0.00039 0.00447 0.00240 0.00687 2.62593

R34 3.79230 0.00005 0.00295 -0.00015 0.00281 3.79511

R35 2.81808 -0.00117 0.00376 -0.00400 -0.00024 2.81784

R36 2.57751 0.00125 0.00042 0.00567 0.00609 2.58360

R37 2.80827 0.00018 0.00004 -0.00086 -0.00082 2.80745

R38 2.74711 -0.00097 -0.00156 -0.00728 -0.00884 2.73827

R39 2.04318 0.00003 0.00028 0.00093 0.00121 2.04438

R40 2.53277 0.00197 0.00081 0.00338 0.00419 2.53696

R41 2.06202 0.00006 0.00050 0.00042 0.00092 2.06294

R42 2.06957 0.00011 0.00119 0.00088 0.00208 2.07165

R43 2.06957 0.00011 0.00119 0.00088 0.00208 2.07165

R44 2.06831 0.00008 0.00114 0.00094 0.00207 2.07039

R45 2.06831 0.00008 0.00114 0.00094 0.00207 2.07039

R46 2.06163 0.00005 0.00035 0.00055 0.00091 2.06254

R47 2.06831 0.00008 0.00114 0.00094 0.00207 2.07039

R48 2.06831 0.00008 0.00114 0.00094 0.00207 2.07039

R49 2.06163 0.00005 0.00035 0.00055 0.00091 2.06254

R50 2.06957 0.00011 0.00119 0.00088 0.00208 2.07165

R51 2.06957 0.00011 0.00119 0.00088 0.00208 2.07165

R52 2.06202 0.00006 0.00050 0.00042 0.00092 2.06294

A1 1.88373 0.00008 -0.00175 0.00084 -0.00092 1.88281

A2 2.20772 -0.00031 -0.00277 -0.00236 -0.00512 2.20260

A3 2.19174 0.00023 0.00452 0.00152 0.00604 2.19777

A4 1.91247 0.00004 0.00031 -0.00045 -0.00015 1.91232

A5 2.18301 -0.00022 -0.00148 -0.00231 -0.00378 2.17924

A6 2.18771 0.00018 0.00117 0.00276 0.00393 2.19163

A7 1.89090 0.00015 0.00188 0.00054 0.00242 1.89332

A8 2.24334 -0.00052 0.00084 -0.00234 -0.00150 2.24184

A9 2.14894 0.00037 -0.00271 0.00180 -0.00091 2.14803

A10 1.85537 -0.00024 -0.00297 -0.00047 -0.00344 1.85193

A11 2.15929 0.00035 -0.00050 0.00106 0.00055 2.15984

A12 2.26853 -0.00011 0.00348 -0.00059 0.00289 2.27142

A13 1.88232 -0.00002 0.00254 -0.00046 0.00209 1.88440

A14 2.17462 0.00007 -0.00188 0.00051 -0.00137 2.17325

A15 2.22625 -0.00005 -0.00066 -0.00005 -0.00072 2.22553

A16 2.14829 0.00022 -0.00210 -0.00165 -0.00377 2.14452

A17 2.22811 0.00015 0.00084 0.00160 0.00244 2.23055

A18 2.16561 -0.00013 -0.00273 -0.00093 -0.00365 2.16196

A19 1.88946 -0.00002 0.00189 -0.00067 0.00121 1.89067

A20 1.91090 -0.00011 0.00005 0.00017 0.00022 1.91112

A21 2.19753 0.00015 0.00124 0.00219 0.00345 2.20098

A22 2.17476 -0.00004 -0.00130 -0.00236 -0.00367 2.17109

A23 1.88615 -0.00003 -0.00154 0.00011 -0.00142 1.88473

A24 2.22771 0.00011 -0.00183 0.00090 -0.00094 2.22677

A25 2.16933 -0.00008 0.00337 -0.00101 0.00236 2.17169

A26 1.85467 0.00018 0.00152 -0.00040 0.00113 1.85579

A27 2.16718 -0.00017 -0.00189 -0.00149 -0.00338 2.16380

A28 2.26134 -0.00001 0.00037 0.00189 0.00225 2.26359

A29 1.88360 -0.00002 -0.00192 0.00079 -0.00113 1.88246

A30 2.17071 -0.00003 -0.00025 -0.00135 -0.00160 2.16911

A31 2.22888 0.00004 0.00218 0.00056 0.00274 2.23161

A32 2.19297 0.00028 0.00539 0.00357 0.00897 2.20194

A33 1.85467 0.00018 0.00152 -0.00040 0.00113 1.85579

A34 2.26134 -0.00001 0.00037 0.00189 0.00225 2.26359

A35 2.16718 -0.00017 -0.00189 -0.00149 -0.00338 2.16380

A36 1.88360 -0.00002 -0.00192 0.00079 -0.00113 1.88246

A37 2.22888 0.00004 0.00218 0.00056 0.00274 2.23161

A38 2.17071 -0.00003 -0.00025 -0.00135 -0.00160 2.16911

A39 1.88946 -0.00002 0.00189 -0.00067 0.00121 1.89067

A40 2.16561 -0.00013 -0.00273 -0.00093 -0.00365 2.16196

A41 2.22811 0.00015 0.00084 0.00160 0.00244 2.23055

A42 1.91090 -0.00011 0.00005 0.00017 0.00022 1.91112

A43 2.19753 0.00015 0.00124 0.00219 0.00345 2.20098

A44 2.17476 -0.00004 -0.00130 -0.00236 -0.00367 2.17109

A45 2.16933 -0.00008 0.00337 -0.00101 0.00236 2.17169

A46 2.22771 0.00011 -0.00183 0.00090 -0.00094 2.22677

A47 1.88615 -0.00003 -0.00154 0.00011 -0.00142 1.88473

A48 2.14829 0.00022 -0.00210 -0.00165 -0.00377 2.14452

A49 1.91247 0.00004 0.00031 -0.00045 -0.00015 1.91232

A50 2.18771 0.00018 0.00117 0.00276 0.00393 2.19163

A51 2.18301 -0.00022 -0.00148 -0.00231 -0.00378 2.17924

A52 2.24334 -0.00052 0.00084 -0.00234 -0.00150 2.24184

A53 2.14894 0.00037 -0.00271 0.00180 -0.00091 2.14803

A54 1.89090 0.00015 0.00188 0.00054 0.00242 1.89332

A55 1.85537 -0.00024 -0.00297 -0.00047 -0.00344 1.85193

A56 2.15929 0.00035 -0.00050 0.00106 0.00055 2.15984

A57 2.26853 -0.00011 0.00348 -0.00059 0.00289 2.27142

A58 1.88232 -0.00002 0.00254 -0.00046 0.00209 1.88440

A59 2.22625 -0.00005 -0.00066 -0.00005 -0.00072 2.22553

A60 2.17462 0.00007 -0.00188 0.00051 -0.00137 2.17325

A61 1.88373 0.00008 -0.00175 0.00084 -0.00092 1.88281

A62 2.20772 -0.00031 -0.00277 -0.00236 -0.00512 2.20260

A63 2.19174 0.00023 0.00452 0.00152 0.00604 2.19777

A64 2.19297 0.00028 0.00539 0.00357 0.00897 2.20194

A65 1.56139 -0.00018 -0.00199 -0.00256 -0.00453 1.55685

A66 1.58021 0.00018 0.00199 0.00256 0.00453 1.58474

A67 1.58021 0.00018 0.00199 0.00256 0.00453 1.58474

A68 1.56139 -0.00018 -0.00199 -0.00256 -0.00453 1.55685

A69 1.94593 -0.00003 0.00078 0.00005 0.00084 1.94677

A70 1.93758 0.00002 0.00006 -0.00085 -0.00079 1.93679

A71 1.93758 0.00002 0.00006 -0.00085 -0.00079 1.93679

A72 1.89244 -0.00002 -0.00002 -0.00036 -0.00037 1.89207

A73 1.89244 -0.00002 -0.00002 -0.00036 -0.00037 1.89207

A74 1.85472 0.00005 -0.00096 0.00249 0.00153 1.85625

A75 1.93735 -0.00008 0.00046 -0.00120 -0.00074 1.93661

A76 1.93735 -0.00008 0.00046 -0.00120 -0.00074 1.93661

A77 1.94339 -0.00004 -0.00055 0.00038 -0.00017 1.94322

A78 1.85831 0.00012 -0.00028 0.00233 0.00206 1.86037

A79 1.89229 0.00005 -0.00006 -0.00009 -0.00015 1.89214

A80 1.89229 0.00005 -0.00006 -0.00009 -0.00015 1.89214

A81 1.93735 -0.00008 0.00046 -0.00120 -0.00074 1.93661

A82 1.93735 -0.00008 0.00046 -0.00120 -0.00074 1.93661

A83 1.94339 -0.00004 -0.00055 0.00038 -0.00017 1.94322

A84 1.85831 0.00012 -0.00028 0.00233 0.00206 1.86037

A85 1.89229 0.00005 -0.00006 -0.00009 -0.00015 1.89214

A86 1.89229 0.00005 -0.00006 -0.00009 -0.00015 1.89214

A87 1.93758 0.00002 0.00006 -0.00085 -0.00079 1.93679

A88 1.93758 0.00002 0.00006 -0.00085 -0.00079 1.93679

A89 1.94593 -0.00003 0.00078 0.00005 0.00084 1.94677

A90 1.85472 0.00005 -0.00096 0.00249 0.00153 1.85625

A91 1.89244 -0.00002 -0.00002 -0.00036 -0.00037 1.89207

A92 1.89244 -0.00002 -0.00002 -0.00036 -0.00037 1.89207

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 1.02951 0.00004 -0.00056 0.00101 0.00045 1.02996

D31 -1.02951 -0.00004 0.00056 -0.00101 -0.00045 -1.02996

D32 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.11208 0.00004 -0.00056 0.00101 0.00045 -2.11164

D34 2.11208 -0.00004 0.00056 -0.00101 -0.00045 2.11164

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 1.03160 0.00002 0.00012 0.00069 0.00081 1.03241

D64 -1.03160 -0.00002 -0.00012 -0.00069 -0.00081 -1.03241

D65 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D66 -2.11000 0.00002 0.00012 0.00069 0.00081 -2.10919

D67 2.11000 -0.00002 -0.00012 -0.00069 -0.00081 2.10919

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 -2.11000 0.00002 0.00012 0.00069 0.00081 -2.10919

D80 2.11000 -0.00002 -0.00012 -0.00069 -0.00081 2.10919

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 1.03160 0.00002 0.00012 0.00069 0.00081 1.03241

D83 -1.03160 -0.00002 -0.00012 -0.00069 -0.00081 -1.03241

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 1.02951 0.00004 -0.00056 0.00101 0.00045 1.02996

D126 -1.02951 -0.00004 0.00056 -0.00101 -0.00045 -1.02996

D127 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D128 -2.11208 0.00004 -0.00056 0.00101 0.00045 -2.11164

D129 2.11208 -0.00004 0.00056 -0.00101 -0.00045 2.11164

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 0.002177 0.000450 NO

RMS Force 0.000394 0.000300 NO

Maximum Displacement 0.012963 0.001800 NO

RMS Displacement 0.002680 0.001200 NO

Predicted change in Energy=-1.100725D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 13:56:35 2019, MaxMem= 2415919104 cpu: 1.4

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.085793 -2.191771 0.000000

2 7 0 -0.734147 -1.869289 0.000000

3 6 0 -0.005694 -2.991573 0.000000

4 6 0 -0.934645 -4.157996 0.000000

5 6 0 -2.198427 -3.636417 0.000000

6 7 0 1.343761 -3.120586 0.000000

7 6 0 2.178351 -2.065067 0.000000

8 7 0 1.855946 -0.758943 0.000000

9 6 0 3.011036 0.001685 0.000000

10 6 0 4.168308 -0.923745 0.000000

11 6 0 3.652553 -2.180100 0.000000

12 7 0 -3.108446 -1.322002 0.000000

13 6 0 -4.168308 0.923745 0.000000

14 6 0 -3.652553 2.180100 0.000000

15 6 0 -2.178351 2.065067 0.000000

16 7 0 -1.855946 0.758943 0.000000

17 6 0 -3.011036 -0.001685 0.000000

18 7 0 -1.343761 3.120586 0.000000

19 7 0 0.734147 1.869289 0.000000

20 6 0 0.005694 2.991573 0.000000

21 6 0 0.934645 4.157996 0.000000

22 6 0 2.198427 3.636417 0.000000

23 6 0 2.085793 2.191771 0.000000

24 7 0 3.108446 1.322002 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.482567 -5.573181 0.000000

27 1 0 -3.134764 -4.178316 0.000000

28 6 0 5.589115 -0.479170 0.000000

29 1 0 4.190173 -3.118109 0.000000

30 6 0 -5.589115 0.479170 0.000000

31 1 0 -4.190173 3.118109 0.000000

32 6 0 0.482567 5.573181 0.000000

33 1 0 3.134764 4.178316 0.000000

34 1 0 -1.327849 -6.263992 0.000000

35 1 0 0.138862 -5.786528 0.877561

36 1 0 0.138862 -5.786528 -0.877561

37 1 0 5.806475 0.138530 0.878377

38 1 0 5.806475 0.138530 -0.878377

39 1 0 6.271735 -1.330809 0.000000

40 1 0 -5.806475 -0.138530 0.878377

41 1 0 -5.806475 -0.138530 -0.878377

42 1 0 -6.271735 1.330809 0.000000

43 1 0 -0.138862 5.786528 0.877561

44 1 0 -0.138862 5.786528 -0.877561

45 1 0 1.327849 6.263992 0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.389584 0.000000

3 C 2.228564 1.337970 0.000000

4 C 2.278418 2.297473 1.491138 0.000000

5 C 1.449031 2.294964 2.285586 1.367184 0.000000

6 N 3.553103 2.425581 1.355608 2.503468 3.579550

7 C 4.266027 2.919071 2.372439 3.751146 4.650305

8 N 4.194080 2.818058 2.906947 4.397836 4.971700

9 C 5.548776 4.186519 4.249735 5.733353 6.354077

10 C 6.381354 4.992807 4.658133 6.041565 6.920543

11 C 5.738359 4.397697 3.747167 4.995444 6.029497

12 N 1.342503 2.436559 3.523426 3.573272 2.486896

13 C 3.747440 4.426568 5.714636 6.023344 4.967445

14 C 4.644135 4.991458 6.328173 6.896267 5.995528

15 C 4.257844 4.191048 5.503639 6.346127 5.701519

16 N 2.959652 2.857628 4.182081 5.002509 4.408683

17 C 2.377510 2.944855 4.239282 4.646109 3.724462

18 N 5.363930 5.026976 6.256909 7.290071 6.810841

19 N 4.944115 4.016572 4.916843 6.254042 6.238012

20 C 5.589398 4.916843 5.983156 7.211142 6.984869

21 C 7.031542 6.254042 7.211142 8.523496 8.400537

22 C 7.233417 6.238012 6.984869 8.400537 8.498615

23 C 6.051245 4.944115 5.589398 7.031542 7.233417

24 N 6.271102 4.994983 5.320225 6.810063 7.262838

25 Zn 3.025623 2.008286 2.991578 4.261748 4.249307

26 C 3.742228 3.712426 2.625283 1.485638 2.587514

27 H 2.246487 3.330851 3.346556 2.200213 1.081842

28 C 7.863664 6.474262 6.133030 7.489539 8.403215

29 H 6.343962 5.080204 4.197774 5.229256 6.409591

30 C 4.405359 5.393141 6.574241 6.570190 5.332431

31 H 5.711675 6.067805 7.405273 7.971209 7.042065

32 C 8.178689 7.541270 8.578660 9.833835 9.591894

33 H 8.236032 7.179276 7.827502 9.276540 9.461131

34 H 4.142157 4.434625 3.529423 2.142389 2.768042

35 H 4.317579 4.108165 2.933051 2.138842 3.294846

36 H 4.317579 4.108165 2.933051 2.138842 3.294846

37 H 8.275853 6.898015 6.659609 8.042038 8.893831

38 H 8.275853 6.898015 6.659609 8.042038 8.893831

39 H 8.401758 7.026545 6.493401 7.741117 8.778353

40 H 4.339449 5.430984 6.523837 6.376707 5.101448

41 H 4.339449 5.430984 6.523837 6.376707 5.101448

42 H 5.470893 6.395742 7.612243 7.655816 6.423797

43 H 8.259171 7.728908 8.822862 10.014836 9.685237

44 H 8.259171 7.728908 8.822862 10.014836 9.685237

45 H 9.118820 8.390596 9.351140 10.664742 10.509650

6 7 8 9 10

6 N 0.000000

7 C 1.345608 0.000000

8 N 2.416545 1.345327 0.000000

9 C 3.539545 2.228189 1.383035 0.000000

10 C 3.578293 2.294023 2.318227 1.481789 0.000000

11 C 2.492998 1.478683 2.290739 2.274143 1.358098

12 N 4.801775 5.338761 4.996221 6.261007 7.287644

13 C 6.836631 7.015204 6.254845 7.238314 8.538875

14 C 7.284259 7.212551 6.243520 7.010629 8.414258

15 C 6.268674 6.003238 4.924489 5.584558 7.015204

16 N 5.028804 4.924489 4.010253 4.925542 6.254845

17 C 5.356473 5.584558 4.925542 6.022074 7.238314

18 N 6.795219 6.268674 5.028804 5.356473 6.836631

19 N 5.026976 4.191048 2.857628 2.944855 4.426568

20 C 6.256909 5.503639 4.182081 4.239282 5.714636

21 C 7.290071 6.346127 5.002509 4.646109 6.023344

22 C 6.810841 5.701519 4.408683 3.724462 4.967445

23 C 5.363930 4.257844 2.959652 2.377510 3.747440

24 N 4.780240 3.512451 2.428804 1.323906 2.483282

25 Zn 3.397610 3.001619 2.005126 3.011037 4.269438

26 C 3.057891 4.403107 5.352152 6.579087 6.576313

27 H 4.601737 5.717956 6.049736 7.432582 7.995443

28 C 5.000011 3.761433 3.743637 2.622539 1.488737

29 H 2.846413 2.270754 3.318776 3.335187 2.194473

30 C 7.811722 8.173535 7.547308 8.613396 9.857762

31 H 8.339409 8.211176 7.182415 7.846624 9.284438

32 C 8.736317 7.824226 6.479349 6.118393 7.469587

33 H 7.515429 6.316214 5.100187 4.178464 5.205693

34 H 4.125349 5.470322 6.359412 7.621327 7.663288

35 H 3.054364 4.333463 5.384710 6.520959 6.375987

36 H 3.054364 4.333463 5.384710 6.520959 6.375987

37 H 5.595462 4.334820 4.145320 2.933385 2.140926

38 H 5.595462 4.334820 4.145320 2.933385 2.140926

39 H 5.242922 4.158717 4.452664 3.522456 2.142453

40 H 7.796799 8.260783 7.737516 8.862263 10.044123

41 H 7.796799 8.260783 7.737516 8.862263 10.044123

42 H 8.821037 9.106917 8.392036 9.377442 10.680708

43 H 9.072208 8.233294 6.898737 6.645027 8.021820

44 H 9.072208 8.233294 6.898737 6.645027 8.021820

45 H 9.384592 8.372370 7.042763 6.484568 7.728633

11 12 13 14 15

11 C 0.000000

12 N 6.815236 0.000000

13 C 8.414258 2.483282 0.000000

14 C 8.507404 3.544118 1.358098 0.000000

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16 N 6.243520 2.428804 2.318227 2.290739 1.345327

17 C 7.010629 1.323906 1.481789 2.274143 2.228189

18 N 7.284259 4.780240 3.578293 2.492998 1.345608

19 N 4.991458 4.994983 4.992807 4.397697 2.919071

20 C 6.328173 5.320225 4.658133 3.747167 2.372439

21 C 6.896267 6.810063 6.041565 4.995444 3.751146

22 C 5.995528 7.262838 6.920543 6.029497 4.650305

23 C 4.644135 6.271102 6.381354 5.738359 4.266027

24 N 3.544118 6.755775 7.287644 6.815236 5.338761

25 Zn 4.253702 3.377887 4.269438 4.253702 3.001619

26 C 5.349039 4.996775 7.469587 8.376287 7.824226

27 H 7.075348 2.856436 5.205693 6.379464 6.316214

28 C 2.577486 8.738302 9.857762 9.616660 8.173535

29 H 1.081155 7.516371 9.284438 9.464638 8.211176

30 C 9.616660 3.065606 1.488737 2.577486 3.761433

31 H 9.464638 4.569980 2.194473 1.081155 2.270754

32 C 8.376287 7.774247 6.576313 5.349039 4.403107

33 H 6.379464 8.320527 7.995443 7.075348 5.717956

34 H 6.440698 5.252979 7.728633 8.758250 8.372370

35 H 5.111014 5.589912 8.021820 8.866347 8.233294

36 H 5.111014 5.589912 8.021820 8.866347 8.233294

37 H 3.284352 9.076371 10.044123 9.716623 8.260783

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39 H 2.753435 9.380185 10.680708 10.527012 9.106917

40 H 9.716623 3.074331 2.140926 3.284352 4.334820

41 H 9.716623 3.074331 2.140926 3.284352 4.334820

42 H 10.527012 4.128414 2.142453 2.753435 4.158717

43 H 8.866347 7.753692 6.375987 5.111014 4.333463

44 H 8.866347 7.753692 6.375987 5.111014 4.333463

45 H 8.758250 8.787947 7.663288 6.440698 5.470322

16 17 18 19 20

16 N 0.000000

17 C 1.383035 0.000000

18 N 2.416545 3.539545 0.000000

19 N 2.818058 4.186519 2.425581 0.000000

20 C 2.906947 4.249735 1.355608 1.337970 0.000000

21 C 4.397836 5.733353 2.503468 2.297473 1.491138

22 C 4.971700 6.354077 3.579550 2.294964 2.285586

23 C 4.194080 5.548776 3.553103 1.389584 2.228564

24 N 4.996221 6.261007 4.801775 2.436559 3.523426

25 Zn 2.005126 3.011037 3.397610 2.008286 2.991578

26 C 6.479349 6.118393 8.736317 7.541270 8.578660

27 H 5.100187 4.178464 7.515429 7.179276 7.827502

28 C 7.547308 8.613396 7.811722 5.393141 6.574241

29 H 7.182415 7.846624 8.339409 6.067805 7.405273

30 C 3.743637 2.622539 5.000011 6.474262 6.133030

31 H 3.318776 3.335187 2.846413 5.080204 4.197774

32 C 5.352152 6.579087 3.057891 3.712426 2.625283

33 H 6.049736 7.432582 4.601737 3.330851 3.346556

34 H 7.042763 6.484568 9.384592 8.390596 9.351140

35 H 6.898737 6.645027 9.072208 7.728908 8.822862

36 H 6.898737 6.645027 9.072208 7.728908 8.822862

37 H 7.737516 8.862263 7.796799 5.430984 6.523837

38 H 7.737516 8.862263 7.796799 5.430984 6.523837

39 H 8.392036 9.377442 8.821037 6.395742 7.612243

40 H 4.145320 2.933385 5.595462 6.898015 6.659609

41 H 4.145320 2.933385 5.595462 6.898015 6.659609

42 H 4.452664 3.522456 5.242922 7.026545 6.493401

43 H 5.384710 6.520959 3.054364 4.108165 2.933051

44 H 5.384710 6.520959 3.054364 4.108165 2.933051

45 H 6.359412 7.621327 4.125349 4.434625 3.529423

21 22 23 24 25

21 C 0.000000

22 C 1.367184 0.000000

23 C 2.278418 1.449031 0.000000

24 N 3.573272 2.486896 1.342503 0.000000

25 Zn 4.261748 4.249307 3.025623 3.377887 0.000000

26 C 9.833835 9.591894 8.178689 7.774247 5.594034

27 H 9.276540 9.461131 8.236032 8.320527 5.223512

28 C 6.570190 5.332431 4.405359 3.065606 5.609617

29 H 7.971209 7.042065 5.711675 4.569980 5.223040

30 C 7.489539 8.403215 7.863664 8.738302 5.609617

31 H 5.229256 6.409591 6.343962 7.516371 5.223040

32 C 1.485638 2.587514 3.742228 4.996775 5.594034

33 H 2.200213 1.081842 2.246487 2.856436 5.223512

34 H 10.664742 10.509650 9.118820 8.787947 6.403185

35 H 10.014836 9.685237 8.259171 7.753692 5.854341

36 H 10.014836 9.685237 8.259171 7.753692 5.854341

37 H 6.376707 5.101448 4.339449 3.074331 5.874171

38 H 6.376707 5.101448 4.339449 3.074331 5.874171

39 H 7.655816 6.423797 5.470893 4.128414 6.411374

40 H 8.042038 8.893831 8.275853 9.076371 5.874171

41 H 8.042038 8.893831 8.275853 9.076371 5.874171

42 H 7.741117 8.778353 8.401758 9.380185 6.411374

43 H 2.138842 3.294846 4.317579 5.589912 5.854341

44 H 2.138842 3.294846 4.317579 5.589912 5.854341

45 H 2.142389 2.768042 4.142157 5.252979 6.403185

26 27 28 29 30

26 C 0.000000

27 H 2.996631 0.000000

28 C 7.925545 9.475745 0.000000

29 H 5.278435 7.401266 2.986811 0.000000

30 C 7.918824 5.264600 11.219235 10.419927 0.000000

31 H 9.449066 7.372361 10.419927 10.446081 2.986811

32 C 11.188068 10.400807 7.918824 9.449066 7.925545

33 H 10.400807 10.447023 5.264600 7.372361 9.475745

34 H 1.091660 2.759526 9.017126 6.351783 7.976755

35 H 1.096269 3.751412 7.657899 4.929877 8.534565

36 H 1.096269 3.751412 7.657899 4.929877 8.534565

37 H 8.540915 9.967570 1.095602 3.740277 11.434467

38 H 8.540915 9.967570 1.095602 3.740277 11.434467

39 H 7.976109 9.828048 1.091448 2.743600 11.998157

40 H 7.658392 4.922343 11.434467 10.468161 1.095602

41 H 7.658392 4.922343 11.434467 10.468161 1.095602

42 H 9.009969 6.339641 11.998157 11.368570 1.091448

43 H 11.398738 10.442397 8.534565 9.939981 7.657899

44 H 11.398738 10.442397 8.534565 9.939981 7.657899

45 H 11.974818 11.355911 7.976755 9.809012 9.017126

31 32 33 34 35

31 H 0.000000

32 C 5.278435 0.000000

33 H 7.401266 2.996631 0.000000

34 H 9.809012 11.974818 11.355911 0.000000

35 H 9.939981 11.398738 10.442397 1.774635 0.000000

36 H 9.939981 11.398738 10.442397 1.774635 1.755123

37 H 10.468161 7.658392 4.922343 9.626132 8.199277

38 H 10.468161 7.658392 4.922343 9.626132 8.385193

39 H 11.368570 9.009969 6.339641 9.060352 7.631230

40 H 3.740277 8.540915 9.967570 7.638778 8.200422

41 H 3.740277 8.540915 9.967570 7.638778 8.386312

42 H 2.743600 7.976109 9.828048 9.062175 9.618854

43 H 4.929877 1.096269 3.751412 12.140793 11.576388

44 H 4.929877 1.096269 3.751412 12.140793 11.708681

45 H 6.351783 1.091660 2.759526 12.806371 12.140793

36 37 38 39 40

36 H 0.000000

37 H 8.385193 0.000000

38 H 8.199277 1.756754 0.000000

39 H 7.631230 1.773970 1.773970 0.000000

40 H 8.386312 11.616254 11.748342 12.168658 0.000000

41 H 8.200422 11.748342 11.616254 12.168658 1.756754

42 H 9.618854 12.168658 12.168658 12.822747 1.773970

43 H 11.708681 8.200422 8.386312 9.618854 8.199277

44 H 11.576388 8.386312 8.200422 9.618854 8.385193

45 H 12.140793 7.638778 7.638778 9.062175 9.626132

41 42 43 44 45

41 H 0.000000

42 H 1.773970 0.000000

43 H 8.385193 7.631230 0.000000

44 H 8.199277 7.631230 1.755123 0.000000

45 H 9.626132 9.060352 1.774635 1.774635 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=3 Diff= 3.43D-03

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 -2.818180 1.101023 0.000000

2 7 0 -2.008091 -0.028002 0.000000

3 6 0 -2.771157 -1.127044 0.000000

4 6 0 -4.202409 -0.708700 0.000000

5 6 0 -4.197978 0.658477 0.000000

6 7 0 -2.379801 -2.424932 0.000000

7 6 0 -1.086918 -2.797914 0.000000

8 7 0 0.000000 -2.005126 0.000000

9 6 0 1.141241 -2.786380 0.000000

10 6 0 0.722692 -4.207828 0.000000

11 6 0 -0.635405 -4.205977 0.000000

12 7 0 -2.400197 2.376800 0.000000

13 6 0 -0.722692 4.207828 0.000000

14 6 0 0.635405 4.205977 0.000000

15 6 0 1.086918 2.797914 0.000000

16 7 0 0.000000 2.005126 0.000000

17 6 0 -1.141241 2.786380 0.000000

18 7 0 2.379801 2.424932 0.000000

19 7 0 2.008091 0.028002 0.000000

20 6 0 2.771157 1.127044 0.000000

21 6 0 4.202409 0.708700 0.000000

22 6 0 4.197978 -0.658477 0.000000

23 6 0 2.818180 -1.101023 0.000000

24 7 0 2.400197 -2.376800 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -5.341193 -1.662792 0.000000

27 1 0 -5.053965 1.320041 0.000000

28 6 0 1.671968 -5.354655 0.000000

29 1 0 -1.300138 -5.058635 0.000000

30 6 0 -1.671968 5.354655 0.000000

31 1 0 1.300138 5.058635 0.000000

32 6 0 5.341193 1.662792 0.000000

33 1 0 5.053965 -1.320041 0.000000

34 1 0 -6.300548 -1.141872 0.000000

35 1 0 -5.303455 -2.318740 0.877561

36 1 0 -5.303455 -2.318740 -0.877561

37 1 0 2.325982 -5.322043 0.878377

38 1 0 2.325982 -5.322043 -0.878377

39 1 0 1.142063 -6.308835 0.000000

40 1 0 -2.325982 5.322043 0.878377

41 1 0 -2.325982 5.322043 -0.878377

42 1 0 -1.142063 6.308835 0.000000

43 1 0 5.303455 2.318740 0.877561

44 1 0 5.303455 2.318740 -0.877561

45 1 0 6.300548 1.141872 0.000000

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

Rotational constants (GHZ): 0.1828056 0.1818975 0.0913801

Leave Link 202 at Tue Sep 17 13:56:35 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 101 beta electrons

nuclear repulsion energy 2761.1254943338 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= -0.1142430020 Hartrees.

Nuclear repulsion after empirical dispersion term = 2761.0112513317 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 = 3500

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.10D-08

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 140

GePol: Fraction of low-weight points (<1% of avg) = 4.00%

GePol: Cavity surface area = 382.372 Ang\*\*2

GePol: Cavity volume = 379.725 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0107382722 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2761.0005130595 Hartrees.

Leave Link 301 at Tue Sep 17 13:56:36 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= 15333 LenP2D= 41264.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.85D-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 13:56:36 2019, MaxMem= 2415919104 cpu: 12.9

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 13:56:36 2019, MaxMem= 2415919104 cpu: 1.6

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= -0.000000 -0.000000 0.000000

Rot= 0.999999 -0.000000 -0.000000 -0.001165 Ang= -0.13 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 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0419 S= 1.0139

Leave Link 401 at Tue Sep 17 13:56:38 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= 36750000.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.99D-15 for 3490.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.78D-15 for 3141 3064.

Iteration 1 A^-1\*A deviation from unit magnitude is 8.22D-15 for 3490.

Iteration 1 A^-1\*A deviation from orthogonality is 6.78D-09 for 1761 1747.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.66D-15 for 140.

Iteration 2 A\*A^-1 deviation from orthogonality is 3.10D-15 for 1990 715.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.22D-15 for 715.

Iteration 2 A^-1\*A deviation from orthogonality is 4.44D-16 for 3487 1330.

E= -1275.84043282580

DIIS: error= 5.60D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.84043282580 IErMin= 1 ErrMin= 5.60D-04

ErrMax= 5.60D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.99D-04 BMatP= 6.99D-04

IDIUse=3 WtCom= 9.94D-01 WtEn= 5.60D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.300 Goal= None Shift= 0.000

Gap= 0.396 Goal= None Shift= 0.000

RMSDP=4.71D-05 MaxDP=1.25D-03 OVMax= 2.52D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.71D-05 CP: 1.00D+00

E= -1275.84071913608 Delta-E= -0.000286310277 Rises=F Damp=F

DIIS: error= 3.05D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84071913608 IErMin= 2 ErrMin= 3.05D-04

ErrMax= 3.05D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.46D-05 BMatP= 6.99D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.05D-03

Coeff-Com: 0.132D+00 0.868D+00

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

Coeff: 0.132D+00 0.868D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.086 Goal= None Shift= 0.000

RMSDP=2.27D-05 MaxDP=8.97D-04 DE=-2.86D-04 OVMax= 1.41D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.91D-05 CP: 1.00D+00 1.26D+00

E= -1275.84074180533 Delta-E= -0.000022669255 Rises=F Damp=F

DIIS: error= 5.06D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1275.84074180533 IErMin= 2 ErrMin= 3.05D-04

ErrMax= 5.06D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.23D-04 BMatP= 9.46D-05

IDIUse=3 WtCom= 3.08D-01 WtEn= 6.92D-01

Coeff-Com: -0.775D-02 0.540D+00 0.468D+00

Coeff-En: 0.000D+00 0.214D+00 0.786D+00

Coeff: -0.238D-02 0.315D+00 0.688D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.085 Goal= None Shift= 0.000

RMSDP=2.24D-05 MaxDP=9.06D-04 DE=-2.27D-05 OVMax= 1.27D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.90D-05 CP: 1.00D+00 1.50D+00 7.95D-01

E= -1275.84076240144 Delta-E= -0.000020596103 Rises=F Damp=F

DIIS: error= 4.34D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84076240144 IErMin= 2 ErrMin= 3.05D-04

ErrMax= 4.34D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.23D-04 BMatP= 9.46D-05

IDIUse=3 WtCom= 3.24D-01 WtEn= 6.76D-01

Coeff-Com: -0.940D-02 0.396D-01 0.501D+00 0.469D+00

Coeff-En: 0.000D+00 0.000D+00 0.347D+00 0.653D+00

Coeff: -0.305D-02 0.128D-01 0.397D+00 0.593D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.085 Goal= None Shift= 0.000

RMSDP=1.54D-05 MaxDP=6.37D-04 DE=-2.06D-05 OVMax= 7.51D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.41D-06 CP: 1.00D+00 1.61D+00 1.49D+00 8.33D-01

E= -1275.84079628669 Delta-E= -0.000033885249 Rises=F Damp=F

DIIS: error= 2.44D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84079628669 IErMin= 5 ErrMin= 2.44D-04

ErrMax= 2.44D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.10D-05 BMatP= 9.46D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.44D-03

Coeff-Com: 0.179D-02-0.143D+00 0.101D+00 0.426D+00 0.615D+00

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

Coeff: 0.178D-02-0.143D+00 0.100D+00 0.425D+00 0.616D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.085 Goal= None Shift= 0.000

RMSDP=1.28D-05 MaxDP=5.56D-04 DE=-3.39D-05 OVMax= 9.85D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.80D-06 CP: 1.00D+00 1.78D+00 1.70D+00 1.30D+00 1.06D+00

E= -1275.84081194614 Delta-E= -0.000015659449 Rises=F Damp=F

DIIS: error= 1.49D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84081194614 IErMin= 6 ErrMin= 1.49D-04

ErrMax= 1.49D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.41D-06 BMatP= 2.10D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.49D-03

Coeff-Com: 0.122D-01-0.173D+00-0.356D+00-0.201D+00 0.310D+00 0.141D+01

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

Coeff: 0.122D-01-0.173D+00-0.356D+00-0.200D+00 0.309D+00 0.141D+01

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.085 Goal= None Shift= 0.000

RMSDP=2.66D-05 MaxDP=1.12D-03 DE=-1.57D-05 OVMax= 2.13D-02

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.91D-06 CP: 1.00D+00 2.14D+00 2.47D+00 2.00D+00 2.11D+00

CP: 2.27D+00

E= -1275.84082689788 Delta-E= -0.000014951745 Rises=F Damp=F

DIIS: error= 5.85D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84082689788 IErMin= 7 ErrMin= 5.85D-05

ErrMax= 5.85D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.08D-06 BMatP= 2.41D-06

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

Coeff-Com: 0.747D-02-0.683D-01-0.246D+00-0.268D+00 0.449D-03 0.929D+00

Coeff-Com: 0.646D+00

Coeff: 0.747D-02-0.683D-01-0.246D+00-0.268D+00 0.449D-03 0.929D+00

Coeff: 0.646D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.085 Goal= None Shift= 0.000

RMSDP=1.02D-05 MaxDP=4.24D-04 DE=-1.50D-05 OVMax= 8.17D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 9.75D-07 CP: 1.00D+00 2.27D+00 2.75D+00 2.27D+00 2.51D+00

CP: 3.00D+00 1.27D+00

E= -1275.84082938382 Delta-E= -0.000002485937 Rises=F Damp=F

DIIS: error= 2.61D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84082938382 IErMin= 8 ErrMin= 2.61D-05

ErrMax= 2.61D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.08D-07 BMatP= 1.08D-06

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

Coeff-Com: -0.285D-02 0.602D-01 0.101D+00 0.924D-03-0.143D+00-0.310D+00

Coeff-Com: 0.280D+00 0.101D+01

Coeff: -0.285D-02 0.602D-01 0.101D+00 0.924D-03-0.143D+00-0.310D+00

Coeff: 0.280D+00 0.101D+01

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.085 Goal= None Shift= 0.000

RMSDP=3.93D-06 MaxDP=1.57D-04 DE=-2.49D-06 OVMax= 3.06D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.18D-06 CP: 1.00D+00 2.32D+00 2.86D+00 2.37D+00 2.71D+00

CP: 3.00D+00 1.67D+00 1.42D+00

E= -1275.84083003806 Delta-E= -0.000000654242 Rises=F Damp=F

DIIS: error= 1.27D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84083003806 IErMin= 9 ErrMin= 1.27D-05

ErrMax= 1.27D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.03D-07 BMatP= 3.08D-07

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

Coeff-Com: -0.319D-02 0.417D-01 0.109D+00 0.743D-01-0.545D-01-0.401D+00

Coeff-Com: -0.702D-01 0.466D+00 0.837D+00

Coeff: -0.319D-02 0.417D-01 0.109D+00 0.743D-01-0.545D-01-0.401D+00

Coeff: -0.702D-01 0.466D+00 0.837D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.085 Goal= None Shift= 0.000

RMSDP=2.28D-06 MaxDP=9.34D-05 DE=-6.54D-07 OVMax= 1.75D-03

Cycle 10 Pass 1 IDiag 1:

RMSU= 3.09D-07 CP: 1.00D+00 2.35D+00 2.92D+00 2.42D+00 2.83D+00

CP: 3.00D+00 1.88D+00 1.88D+00 1.50D+00

E= -1275.84083024858 Delta-E= -0.000000210522 Rises=F Damp=F

DIIS: error= 8.65D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84083024858 IErMin=10 ErrMin= 8.65D-06

ErrMax= 8.65D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.19D-08 BMatP= 1.03D-07

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

Coeff-Com: -0.297D-03-0.674D-02 0.165D-01 0.484D-01 0.420D-01-0.887D-01

Coeff-Com: -0.163D+00-0.165D+00 0.387D+00 0.930D+00

Coeff: -0.297D-03-0.674D-02 0.165D-01 0.484D-01 0.420D-01-0.887D-01

Coeff: -0.163D+00-0.165D+00 0.387D+00 0.930D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.085 Goal= None Shift= 0.000

RMSDP=1.03D-06 MaxDP=4.03D-05 DE=-2.11D-07 OVMax= 7.36D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 2.31D-07 CP: 1.00D+00 2.36D+00 2.95D+00 2.45D+00 2.88D+00

CP: 3.00D+00 2.01D+00 2.16D+00 1.86D+00 1.15D+00

E= -1275.84083031118 Delta-E= -0.000000062602 Rises=F Damp=F

DIIS: error= 3.68D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84083031118 IErMin=11 ErrMin= 3.68D-06

ErrMax= 3.68D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.14D-09 BMatP= 3.19D-08

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

Coeff-Com: 0.634D-03-0.129D-01-0.225D-01-0.507D-02 0.218D-01 0.600D-01

Coeff-Com: -0.306D-01-0.134D+00-0.692D-01 0.367D+00 0.825D+00

Coeff: 0.634D-03-0.129D-01-0.225D-01-0.507D-02 0.218D-01 0.600D-01

Coeff: -0.306D-01-0.134D+00-0.692D-01 0.367D+00 0.825D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.085 Goal= None Shift= 0.000

RMSDP=9.27D-07 MaxDP=3.78D-05 DE=-6.26D-08 OVMax= 7.34D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.13D-07 CP: 1.00D+00 2.37D+00 2.97D+00 2.47D+00 2.91D+00

CP: 3.00D+00 2.07D+00 2.27D+00 1.99D+00 1.40D+00

CP: 1.22D+00

E= -1275.84083032963 Delta-E= -0.000000018445 Rises=F Damp=F

DIIS: error= 2.61D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84083032963 IErMin=12 ErrMin= 2.61D-06

ErrMax= 2.61D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.87D-09 BMatP= 9.14D-09

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

Coeff-Com: 0.484D-03-0.584D-02-0.170D-01-0.157D-01 0.179D-02 0.645D-01

Coeff-Com: 0.284D-01-0.398D-01-0.172D+00-0.636D-01 0.524D+00 0.695D+00

Coeff: 0.484D-03-0.584D-02-0.170D-01-0.157D-01 0.179D-02 0.645D-01

Coeff: 0.284D-01-0.398D-01-0.172D+00-0.636D-01 0.524D+00 0.695D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.085 Goal= None Shift= 0.000

RMSDP=1.96D-07 MaxDP=9.30D-06 DE=-1.84D-08 OVMax= 1.25D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 4.81D-08 CP: 1.00D+00 2.37D+00 2.98D+00 2.48D+00 2.92D+00

CP: 3.00D+00 2.09D+00 2.32D+00 2.06D+00 1.53D+00

CP: 1.53D+00 1.08D+00

E= -1275.84083033341 Delta-E= -0.000000003779 Rises=F Damp=F

DIIS: error= 9.33D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84083033341 IErMin=13 ErrMin= 9.33D-07

ErrMax= 9.33D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.54D-10 BMatP= 3.87D-09

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

Coeff-Com: -0.877D-04 0.286D-02 0.366D-02-0.283D-02-0.770D-02-0.296D-02

Coeff-Com: 0.153D-01 0.277D-01-0.208D-01-0.146D+00-0.113D+00 0.204D+00

Coeff-Com: 0.104D+01

Coeff: -0.877D-04 0.286D-02 0.366D-02-0.283D-02-0.770D-02-0.296D-02

Coeff: 0.153D-01 0.277D-01-0.208D-01-0.146D+00-0.113D+00 0.204D+00

Coeff: 0.104D+01

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.085 Goal= None Shift= 0.000

RMSDP=1.93D-07 MaxDP=7.24D-06 DE=-3.78D-09 OVMax= 1.40D-04

Cycle 14 Pass 1 IDiag 1:

RMSU= 2.42D-08 CP: 1.00D+00 2.37D+00 2.98D+00 2.48D+00 2.93D+00

CP: 3.00D+00 2.11D+00 2.37D+00 2.11D+00 1.61D+00

CP: 1.72D+00 1.34D+00 1.20D+00

E= -1275.84083033454 Delta-E= -0.000000001132 Rises=F Damp=F

DIIS: error= 3.43D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84083033454 IErMin=14 ErrMin= 3.43D-07

ErrMax= 3.43D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.10D-10 BMatP= 5.54D-10

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

Coeff-Com: -0.747D-04 0.176D-02 0.270D-02-0.694D-03-0.410D-02-0.588D-02

Coeff-Com: 0.579D-02 0.176D-01 0.351D-02-0.678D-01-0.962D-01 0.276D-01

Coeff-Com: 0.492D+00 0.624D+00

Coeff: -0.747D-04 0.176D-02 0.270D-02-0.694D-03-0.410D-02-0.588D-02

Coeff: 0.579D-02 0.176D-01 0.351D-02-0.678D-01-0.962D-01 0.276D-01

Coeff: 0.492D+00 0.624D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.085 Goal= None Shift= 0.000

RMSDP=6.39D-08 MaxDP=2.52D-06 DE=-1.13D-09 OVMax= 4.99D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 9.71D-09 CP: 1.00D+00 2.37D+00 2.98D+00 2.48D+00 2.93D+00

CP: 3.00D+00 2.11D+00 2.37D+00 2.12D+00 1.62D+00

CP: 1.74D+00 1.39D+00 1.33D+00 1.08D+00

E= -1275.84083033460 Delta-E= -0.000000000059 Rises=F Damp=F

DIIS: error= 1.64D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.84083033460 IErMin=15 ErrMin= 1.64D-07

ErrMax= 1.64D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.17D-11 BMatP= 1.10D-10

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

Coeff-Com: -0.175D-04-0.240D-04 0.660D-03 0.142D-02 0.992D-03-0.369D-02

Coeff-Com: -0.383D-02-0.536D-03 0.121D-01 0.192D-01-0.106D-01-0.742D-01

Coeff-Com: -0.112D+00 0.340D+00 0.830D+00

Coeff: -0.175D-04-0.240D-04 0.660D-03 0.142D-02 0.992D-03-0.369D-02

Coeff: -0.383D-02-0.536D-03 0.121D-01 0.192D-01-0.106D-01-0.742D-01

Coeff: -0.112D+00 0.340D+00 0.830D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.085 Goal= None Shift= 0.000

RMSDP=1.45D-08 MaxDP=9.74D-07 DE=-5.91D-11 OVMax= 7.07D-06

Cycle 16 Pass 1 IDiag 1:

RMSU= 4.80D-09 CP: 1.00D+00 2.37D+00 2.98D+00 2.48D+00 2.93D+00

CP: 3.00D+00 2.12D+00 2.37D+00 2.13D+00 1.63D+00

CP: 1.76D+00 1.41D+00 1.39D+00 1.37D+00 1.04D+00

E= -1275.84083033463 Delta-E= -0.000000000027 Rises=F Damp=F

DIIS: error= 7.62D-08 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1275.84083033463 IErMin=16 ErrMin= 7.62D-08

ErrMax= 7.62D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.02D-12 BMatP= 3.17D-11

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

Coeff-Com: 0.439D-06-0.226D-03-0.792D-04 0.715D-03 0.958D-03-0.111D-02

Coeff-Com: -0.253D-02-0.193D-02 0.528D-02 0.175D-01 0.731D-02-0.438D-01

Coeff-Com: -0.112D+00 0.826D-01 0.404D+00 0.643D+00

Coeff: 0.439D-06-0.226D-03-0.792D-04 0.715D-03 0.958D-03-0.111D-02

Coeff: -0.253D-02-0.193D-02 0.528D-02 0.175D-01 0.731D-02-0.438D-01

Coeff: -0.112D+00 0.826D-01 0.404D+00 0.643D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.085 Goal= None Shift= 0.000

RMSDP=7.38D-09 MaxDP=3.48D-07 DE=-2.68D-11 OVMax= 5.21D-06

Error on total polarization charges = 0.06472

SCF Done: E(UB3LYP) = -1275.84083033 A.U. after 16 cycles

NFock= 16 Conv=0.74D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0391 S= 1.0130

<L.S>= 0.000000000000E+00

KE= 1.320777112667D+03 PE=-8.573936624700D+03 EE= 3.216318168639D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.74

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0391, after 2.0009

Leave Link 502 at Tue Sep 17 13:58:09 2019, MaxMem= 2415919104 cpu: 1602.0

(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= 15333 LenP2D= 41264.

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 = 245

Leave Link 701 at Tue Sep 17 13:58:13 2019, MaxMem= 2415919104 cpu: 70.9

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 13:58:13 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 13:58:24 2019, MaxMem= 2415919104 cpu: 202.3

(Enter /home/blab/g09/l716.exe)

Dipole =-2.36255460D-13-1.31894495D-13 1.11022302D-15

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.006091135 -0.002143711 0.000000000

2 7 -0.003553610 0.001612229 -0.000000000

3 6 -0.001660297 -0.004724719 0.000000000

4 6 0.002375589 0.002902736 0.000000000

5 6 -0.001691447 0.000462942 -0.000000000

6 7 0.003268261 0.003319563 -0.000000000

7 6 -0.001736632 -0.005946452 0.000000000

8 7 0.001083402 0.003881692 -0.000000000

9 6 -0.003612341 0.001527539 0.000000000

10 6 0.001361105 -0.002091841 0.000000000

11 6 0.000780529 0.001788814 -0.000000000

12 7 -0.004258739 0.003253162 -0.000000000

13 6 -0.001361105 0.002091841 -0.000000000

14 6 -0.000780529 -0.001788814 -0.000000000

15 6 0.001736632 0.005946452 -0.000000000

16 7 -0.001083402 -0.003881692 -0.000000000

17 6 0.003612341 -0.001527539 -0.000000000

18 7 -0.003268261 -0.003319563 0.000000000

19 7 0.003553610 -0.001612229 0.000000000

20 6 0.001660297 0.004724719 -0.000000000

21 6 -0.002375589 -0.002902736 0.000000000

22 6 0.001691447 -0.000462942 0.000000000

23 6 -0.006091135 0.002143711 -0.000000000

24 7 0.004258739 -0.003253162 -0.000000000

25 30 -0.000000000 0.000000000 0.000000000

26 6 0.000255209 -0.000575610 -0.000000000

27 1 0.000414889 -0.000003647 -0.000000000

28 6 -0.000044162 0.000125483 -0.000000000

29 1 0.000067271 0.000053502 0.000000000

30 6 0.000044162 -0.000125483 -0.000000000

31 1 -0.000067271 -0.000053502 0.000000000

32 6 -0.000255209 0.000575610 0.000000000

33 1 -0.000414889 0.000003647 0.000000000

34 1 0.000168750 0.000160814 -0.000000000

35 1 -0.000295994 -0.000028749 -0.000521603

36 1 -0.000295994 -0.000028749 0.000521603

37 1 -0.000215041 -0.000306204 -0.000574463

38 1 -0.000215041 -0.000306204 0.000574463

39 1 -0.000234810 0.000177557 -0.000000000

40 1 0.000215041 0.000306204 -0.000574463

41 1 0.000215041 0.000306204 0.000574463

42 1 0.000234810 -0.000177557 0.000000000

43 1 0.000295994 0.000028749 -0.000521603

44 1 0.000295994 0.000028749 0.000521603

45 1 -0.000168750 -0.000160814 -0.000000000

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

Cartesian Forces: Max 0.006091135 RMS 0.001853937

Leave Link 716 at Tue Sep 17 13:58:24 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 0.003796470 RMS 0.000706792

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= -9.08D-05 DEPred=-1.10D-04 R= 8.25D-01

TightC=F SS= 1.41D+00 RLast= 4.51D-02 DXNew= 5.0454D-01 1.3532D-01

Trust test= 8.25D-01 RLast= 4.51D-02 DXMaxT set to 3.00D-01

ITU= 1 1 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01340

Eigenvalues --- 0.01342 0.01344 0.01345 0.01604 0.01622

Eigenvalues --- 0.01635 0.01636 0.01775 0.01791 0.01815

Eigenvalues --- 0.01817 0.01891 0.01907 0.01941 0.01947

Eigenvalues --- 0.01998 0.01999 0.02043 0.02050 0.02070

Eigenvalues --- 0.02088 0.02103 0.02112 0.02114 0.02205

Eigenvalues --- 0.02311 0.02319 0.02351 0.02373 0.06338

Eigenvalues --- 0.07177 0.07177 0.07211 0.07211 0.07355

Eigenvalues --- 0.07358 0.07362 0.07551 0.14487 0.14511

Eigenvalues --- 0.15854 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16003 0.16014 0.16068

Eigenvalues --- 0.16143 0.16776 0.18473 0.22066 0.22093

Eigenvalues --- 0.22603 0.23840 0.23853 0.23885 0.24265

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25010 0.25190

Eigenvalues --- 0.25618 0.29892 0.32244 0.33195 0.33197

Eigenvalues --- 0.33282 0.33282 0.33313 0.33346 0.33639

Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33730 0.34383 0.34437 0.34437

Eigenvalues --- 0.34439 0.34933 0.35553 0.35564 0.35608

Eigenvalues --- 0.35682 0.35682 0.35750 0.37894 0.39223

Eigenvalues --- 0.40635 0.41696 0.41765 0.41904 0.47875

Eigenvalues --- 0.48932 0.49019 0.49029 0.51015 0.51356

Eigenvalues --- 0.51363 0.51401 0.53994 0.54042 0.54340

Eigenvalues --- 0.56300 0.56354 0.56362 0.98339

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 0.89663 0.10337

Cosine: 1.000 > 0.970

Length: 1.000

GDIIS step was calculated using 2 of the last 5 vectors.

Iteration 1 RMS(Cart)= 0.00236642 RMS(Int)= 0.00000354

Iteration 2 RMS(Cart)= 0.00000455 RMS(Int)= 0.00000099

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000099

ITry= 1 IFail=0 DXMaxC= 9.12D-03 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.14D-09 for atom 27.

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

(Linear) (Quad) (Total)

R1 2.62593 -0.00231 -0.00071 -0.00020 -0.00090 2.62503

R2 2.73827 -0.00058 0.00091 -0.00740 -0.00648 2.73179

R3 2.53696 0.00380 -0.00043 0.00788 0.00745 2.54442

R4 2.52840 0.00216 0.00073 -0.00025 0.00048 2.52888

R5 3.79511 -0.00011 -0.00029 0.00258 0.00229 3.79740

R6 2.81784 -0.00264 0.00002 -0.00668 -0.00665 2.81119

R7 2.56173 0.00136 -0.00100 0.00814 0.00714 2.56887

R8 2.58360 0.00070 -0.00063 0.00714 0.00651 2.59011

R9 2.80745 0.00040 0.00008 0.00083 0.00091 2.80836

R10 2.04438 -0.00036 -0.00012 0.00081 0.00069 2.04507

R11 2.54283 -0.00327 0.00060 -0.00938 -0.00878 2.53405

R12 2.54230 0.00282 0.00053 0.00133 0.00185 2.54415

R13 2.79431 0.00018 -0.00082 0.00519 0.00437 2.79867

R14 2.61356 -0.00162 -0.00061 0.00041 -0.00020 2.61336

R15 3.78914 -0.00011 0.00001 -0.00036 -0.00036 3.78878

R16 2.80018 0.00162 -0.00042 0.00552 0.00511 2.80528

R17 2.50182 -0.00126 0.00112 -0.00906 -0.00794 2.49388

R18 2.56643 -0.00156 0.00025 -0.00216 -0.00191 2.56453

R19 2.81331 -0.00077 -0.00020 0.00123 0.00103 2.81434

R20 2.04309 -0.00001 -0.00001 0.00029 0.00028 2.04337

R21 2.50182 -0.00126 0.00112 -0.00906 -0.00794 2.49388

R22 2.56643 -0.00156 0.00025 -0.00216 -0.00191 2.56453

R23 2.80018 0.00162 -0.00042 0.00552 0.00511 2.80528

R24 2.81331 -0.00077 -0.00020 0.00123 0.00103 2.81434

R25 2.79431 0.00018 -0.00082 0.00519 0.00437 2.79867

R26 2.04309 -0.00001 -0.00001 0.00029 0.00028 2.04337

R27 2.54230 0.00282 0.00053 0.00133 0.00185 2.54415

R28 2.54283 -0.00327 0.00060 -0.00938 -0.00878 2.53405

R29 2.61356 -0.00162 -0.00061 0.00041 -0.00020 2.61336

R30 3.78914 -0.00011 0.00001 -0.00036 -0.00036 3.78878

R31 2.56173 0.00136 -0.00100 0.00814 0.00714 2.56887

R32 2.52840 0.00216 0.00073 -0.00025 0.00048 2.52888

R33 2.62593 -0.00231 -0.00071 -0.00020 -0.00090 2.62503

R34 3.79511 -0.00011 -0.00029 0.00258 0.00229 3.79740

R35 2.81784 -0.00264 0.00002 -0.00668 -0.00665 2.81119

R36 2.58360 0.00070 -0.00063 0.00714 0.00651 2.59011

R37 2.80745 0.00040 0.00008 0.00083 0.00091 2.80836

R38 2.73827 -0.00058 0.00091 -0.00740 -0.00648 2.73179

R39 2.04438 -0.00036 -0.00012 0.00081 0.00069 2.04507

R40 2.53696 0.00380 -0.00043 0.00788 0.00745 2.54442

R41 2.06294 -0.00023 -0.00009 0.00083 0.00073 2.06367

R42 2.07165 -0.00058 -0.00021 0.00172 0.00150 2.07315

R43 2.07165 -0.00058 -0.00021 0.00172 0.00150 2.07315

R44 2.07039 -0.00068 -0.00021 0.00170 0.00148 2.07187

R45 2.07039 -0.00068 -0.00021 0.00170 0.00148 2.07187

R46 2.06254 -0.00028 -0.00009 0.00078 0.00069 2.06323

R47 2.07039 -0.00068 -0.00021 0.00170 0.00148 2.07187

R48 2.07039 -0.00068 -0.00021 0.00170 0.00148 2.07187

R49 2.06254 -0.00028 -0.00009 0.00078 0.00069 2.06323

R50 2.07165 -0.00058 -0.00021 0.00172 0.00150 2.07315

R51 2.07165 -0.00058 -0.00021 0.00172 0.00150 2.07315

R52 2.06294 -0.00023 -0.00009 0.00083 0.00073 2.06367

A1 1.88281 0.00031 0.00009 0.00045 0.00055 1.88336

A2 2.20260 0.00015 0.00053 -0.00348 -0.00294 2.19966

A3 2.19777 -0.00046 -0.00062 0.00302 0.00240 2.20017

A4 1.91232 -0.00003 0.00002 -0.00099 -0.00097 1.91135

A5 2.17924 0.00019 0.00039 -0.00225 -0.00186 2.17738

A6 2.19163 -0.00016 -0.00041 0.00324 0.00283 2.19446

A7 1.89332 -0.00030 -0.00025 0.00232 0.00207 1.89539

A8 2.24184 -0.00055 0.00016 -0.00476 -0.00460 2.23724

A9 2.14803 0.00085 0.00009 0.00244 0.00253 2.15056

A10 1.85193 0.00027 0.00036 -0.00262 -0.00226 1.84967

A11 2.15984 0.00047 -0.00006 0.00315 0.00309 2.16294

A12 2.27142 -0.00074 -0.00030 -0.00054 -0.00083 2.27058

A13 1.88440 -0.00026 -0.00022 0.00083 0.00061 1.88502

A14 2.17325 0.00034 0.00014 0.00025 0.00039 2.17364

A15 2.22553 -0.00009 0.00007 -0.00108 -0.00100 2.22453

A16 2.14452 0.00052 0.00039 0.00136 0.00175 2.14628

A17 2.23055 0.00024 -0.00025 0.00094 0.00068 2.23123

A18 2.16196 0.00030 0.00038 -0.00136 -0.00098 2.16098

A19 1.89067 -0.00055 -0.00013 0.00042 0.00030 1.89097

A20 1.91112 -0.00010 -0.00002 -0.00002 -0.00005 1.91108

A21 2.20098 -0.00024 -0.00036 0.00179 0.00144 2.20241

A22 2.17109 0.00033 0.00038 -0.00177 -0.00139 2.16970

A23 1.88473 -0.00005 0.00015 -0.00054 -0.00039 1.88433

A24 2.22677 0.00069 0.00010 -0.00003 0.00006 2.22683

A25 2.17169 -0.00064 -0.00024 0.00057 0.00033 2.17202

A26 1.85579 0.00039 -0.00012 0.00093 0.00082 1.85661

A27 2.16380 -0.00012 0.00035 -0.00204 -0.00169 2.16212

A28 2.26359 -0.00027 -0.00023 0.00110 0.00087 2.26446

A29 1.88246 0.00030 0.00012 -0.00079 -0.00068 1.88179

A30 2.16911 -0.00006 0.00017 -0.00075 -0.00058 2.16853

A31 2.23161 -0.00024 -0.00028 0.00154 0.00125 2.23287

A32 2.20194 -0.00118 -0.00093 0.00496 0.00403 2.20597

A33 1.85579 0.00039 -0.00012 0.00093 0.00082 1.85661

A34 2.26359 -0.00027 -0.00023 0.00110 0.00087 2.26446

A35 2.16380 -0.00012 0.00035 -0.00204 -0.00169 2.16212

A36 1.88246 0.00030 0.00012 -0.00079 -0.00068 1.88179

A37 2.23161 -0.00024 -0.00028 0.00154 0.00125 2.23287

A38 2.16911 -0.00006 0.00017 -0.00075 -0.00058 2.16853

A39 1.89067 -0.00055 -0.00013 0.00042 0.00030 1.89097

A40 2.16196 0.00030 0.00038 -0.00136 -0.00098 2.16098

A41 2.23055 0.00024 -0.00025 0.00094 0.00068 2.23123

A42 1.91112 -0.00010 -0.00002 -0.00002 -0.00005 1.91108

A43 2.20098 -0.00024 -0.00036 0.00179 0.00144 2.20241

A44 2.17109 0.00033 0.00038 -0.00177 -0.00139 2.16970

A45 2.17169 -0.00064 -0.00024 0.00057 0.00033 2.17202

A46 2.22677 0.00069 0.00010 -0.00003 0.00006 2.22683

A47 1.88473 -0.00005 0.00015 -0.00054 -0.00039 1.88433

A48 2.14452 0.00052 0.00039 0.00136 0.00175 2.14628

A49 1.91232 -0.00003 0.00002 -0.00099 -0.00097 1.91135

A50 2.19163 -0.00016 -0.00041 0.00324 0.00283 2.19446

A51 2.17924 0.00019 0.00039 -0.00225 -0.00186 2.17738

A52 2.24184 -0.00055 0.00016 -0.00476 -0.00460 2.23724

A53 2.14803 0.00085 0.00009 0.00244 0.00253 2.15056

A54 1.89332 -0.00030 -0.00025 0.00232 0.00207 1.89539

A55 1.85193 0.00027 0.00036 -0.00262 -0.00226 1.84967

A56 2.15984 0.00047 -0.00006 0.00315 0.00309 2.16294

A57 2.27142 -0.00074 -0.00030 -0.00054 -0.00083 2.27058

A58 1.88440 -0.00026 -0.00022 0.00083 0.00061 1.88502

A59 2.22553 -0.00009 0.00007 -0.00108 -0.00100 2.22453

A60 2.17325 0.00034 0.00014 0.00025 0.00039 2.17364

A61 1.88281 0.00031 0.00009 0.00045 0.00055 1.88336

A62 2.20260 0.00015 0.00053 -0.00348 -0.00294 2.19966

A63 2.19777 -0.00046 -0.00062 0.00302 0.00240 2.20017

A64 2.20194 -0.00118 -0.00093 0.00496 0.00403 2.20597

A65 1.55685 0.00018 0.00047 -0.00257 -0.00210 1.55475

A66 1.58474 -0.00018 -0.00047 0.00257 0.00210 1.58684

A67 1.58474 -0.00018 -0.00047 0.00257 0.00210 1.58684

A68 1.55685 0.00018 0.00047 -0.00257 -0.00210 1.55475

A69 1.94677 -0.00011 -0.00009 -0.00066 -0.00075 1.94602

A70 1.93679 0.00020 0.00008 -0.00014 -0.00006 1.93673

A71 1.93679 0.00020 0.00008 -0.00014 -0.00006 1.93673

A72 1.89207 -0.00007 0.00004 -0.00072 -0.00069 1.89138

A73 1.89207 -0.00007 0.00004 -0.00072 -0.00069 1.89138

A74 1.85625 -0.00017 -0.00016 0.00251 0.00235 1.85860

A75 1.93661 -0.00007 0.00008 -0.00104 -0.00097 1.93564

A76 1.93661 -0.00007 0.00008 -0.00104 -0.00097 1.93564

A77 1.94322 -0.00004 0.00002 -0.00087 -0.00086 1.94236

A78 1.86037 -0.00001 -0.00021 0.00275 0.00254 1.86290

A79 1.89214 0.00010 0.00002 0.00021 0.00022 1.89236

A80 1.89214 0.00010 0.00002 0.00021 0.00022 1.89236

A81 1.93661 -0.00007 0.00008 -0.00104 -0.00097 1.93564

A82 1.93661 -0.00007 0.00008 -0.00104 -0.00097 1.93564

A83 1.94322 -0.00004 0.00002 -0.00087 -0.00086 1.94236

A84 1.86037 -0.00001 -0.00021 0.00275 0.00254 1.86290

A85 1.89214 0.00010 0.00002 0.00021 0.00022 1.89236

A86 1.89214 0.00010 0.00002 0.00021 0.00022 1.89236

A87 1.93679 0.00020 0.00008 -0.00014 -0.00006 1.93673

A88 1.93679 0.00020 0.00008 -0.00014 -0.00006 1.93673

A89 1.94677 -0.00011 -0.00009 -0.00066 -0.00075 1.94602

A90 1.85625 -0.00017 -0.00016 0.00251 0.00235 1.85860

A91 1.89207 -0.00007 0.00004 -0.00072 -0.00069 1.89138

A92 1.89207 -0.00007 0.00004 -0.00072 -0.00069 1.89138

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

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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

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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 1.02996 0.00002 -0.00005 0.00147 0.00143 1.03138

D31 -1.02996 -0.00002 0.00005 -0.00147 -0.00143 -1.03138

D32 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.11164 0.00002 -0.00005 0.00147 0.00143 -2.11021

D34 2.11164 -0.00002 0.00005 -0.00147 -0.00143 2.11021

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

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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

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 1.03241 -0.00005 -0.00008 0.00105 0.00096 1.03337

D64 -1.03241 0.00005 0.00008 -0.00105 -0.00096 -1.03337

D65 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D66 -2.10919 -0.00005 -0.00008 0.00105 0.00096 -2.10822

D67 2.10919 0.00005 0.00008 -0.00105 -0.00096 2.10822

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 -2.10919 -0.00005 -0.00008 0.00105 0.00096 -2.10822

D80 2.10919 0.00005 0.00008 -0.00105 -0.00096 2.10822

D81 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D82 1.03241 -0.00005 -0.00008 0.00105 0.00096 1.03337

D83 -1.03241 0.00005 0.00008 -0.00105 -0.00096 -1.03337

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 1.02996 0.00002 -0.00005 0.00147 0.00143 1.03138

D126 -1.02996 -0.00002 0.00005 -0.00147 -0.00143 -1.03138

D127 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D128 -2.11164 0.00002 -0.00005 0.00147 0.00143 -2.11021

D129 2.11164 -0.00002 0.00005 -0.00147 -0.00143 2.11021

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 0.003796 0.000450 NO

RMS Force 0.000707 0.000300 NO

Maximum Displacement 0.009115 0.001800 NO

RMS Displacement 0.002365 0.001200 NO

Predicted change in Energy=-1.155155D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 13:58:24 2019, MaxMem= 2415919104 cpu: 1.7

(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 -2.083446 -2.193058 0.000000

2 7 0 -0.732096 -1.871396 0.000000

3 6 0 -0.005185 -2.994982 0.000000

4 6 0 -0.931271 -4.159188 0.000000

5 6 0 -2.197355 -3.634164 0.000000

6 7 0 1.348427 -3.120149 0.000000

7 6 0 2.178710 -2.067150 0.000000

8 7 0 1.855191 -0.760292 0.000000

9 6 0 3.009715 0.001001 0.000000

10 6 0 4.169313 -0.925848 0.000000

11 6 0 3.655259 -2.181810 0.000000

12 7 0 -3.106072 -1.317184 0.000000

13 6 0 -4.169313 0.925848 0.000000

14 6 0 -3.655259 2.181810 0.000000

15 6 0 -2.178710 2.067150 0.000000

16 7 0 -1.855191 0.760292 0.000000

17 6 0 -3.009715 -0.001001 0.000000

18 7 0 -1.348427 3.120149 0.000000

19 7 0 0.732096 1.871396 0.000000

20 6 0 0.005185 2.994982 0.000000

21 6 0 0.931271 4.159188 0.000000

22 6 0 2.197355 3.634164 0.000000

23 6 0 2.083446 2.193058 0.000000

24 7 0 3.106072 1.317184 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.482611 -5.575967 0.000000

27 1 0 -3.134373 -4.175609 0.000000

28 6 0 5.589784 -0.478384 0.000000

29 1 0 4.192761 -3.120059 0.000000

30 6 0 -5.589784 0.478384 0.000000

31 1 0 -4.192761 3.120059 0.000000

32 6 0 0.482611 5.575967 0.000000

33 1 0 3.134373 4.175609 0.000000

34 1 0 -1.330447 -6.264257 0.000000

35 1 0 0.137528 -5.791352 0.878969

36 1 0 0.137528 -5.791352 -0.878969

37 1 0 5.805363 0.139254 0.879836

38 1 0 5.805363 0.139254 -0.879836

39 1 0 6.273536 -1.329582 0.000000

40 1 0 -5.805363 -0.139254 0.879836

41 1 0 -5.805363 -0.139254 -0.879836

42 1 0 -6.273536 1.329582 0.000000

43 1 0 -0.137528 5.791352 0.878969

44 1 0 -0.137528 5.791352 -0.878969

45 1 0 1.330447 6.264257 0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.389106 0.000000

3 C 2.227611 1.338225 0.000000

4 C 2.278853 2.296446 1.487619 0.000000

5 C 1.445600 2.292233 2.283453 1.370627 0.000000

6 N 3.554891 2.426512 1.359387 2.505319 3.582845

7 C 4.264015 2.917381 2.372819 3.748147 4.648169

8 N 4.191143 2.815778 2.907721 4.395095 4.968125

9 C 5.545645 4.184139 4.250357 5.730492 6.350432

10 C 6.379876 4.991781 4.659158 6.039077 6.918774

11 C 5.738717 4.398323 3.749680 4.994626 6.030126

12 N 1.346447 2.437809 3.525693 3.578651 2.488807

13 C 3.752122 4.431595 5.719517 6.028475 4.968131

14 C 4.648663 4.997335 6.334210 6.901330 5.995918

15 C 4.261273 4.195811 5.509028 6.350069 5.701344

16 N 2.962158 2.861315 4.186240 5.005488 4.407756

17 C 2.379725 2.947189 4.241595 4.648704 3.722876

18 N 5.363807 5.029451 6.260921 7.291280 6.807453

19 N 4.944397 4.018998 4.921912 6.255776 6.236415

20 C 5.592687 4.921912 5.989973 7.215199 6.985467

21 C 7.031326 6.255776 7.215199 8.524344 8.397894

22 C 7.230613 6.236415 6.985467 8.397894 8.493648

23 C 6.049877 4.944397 5.592687 7.031326 7.230613

24 N 6.265214 4.989847 5.317396 6.803734 7.255493

25 Zn 3.024938 2.009499 2.994987 4.262172 4.246824

26 C 3.742558 3.712962 2.624770 1.486122 2.590549

27 H 2.243871 3.328714 3.344503 2.203163 1.082205

28 C 7.862478 6.473534 6.134896 7.488156 8.402290

29 H 6.344297 5.080686 4.199809 5.228335 6.410763

30 C 4.408061 5.396164 6.576626 6.573340 5.331193

31 H 5.716504 6.073782 7.411445 7.976512 7.042810

32 C 8.181833 7.545775 8.584819 9.837291 9.592117

33 H 8.233199 7.177454 7.827784 9.273527 9.456208

34 H 4.140250 4.433425 3.527673 2.142582 2.769282

35 H 4.318915 4.110339 2.934729 2.139831 3.298139

36 H 4.318915 4.110339 2.934729 2.139831 3.298139

37 H 8.273277 6.896028 6.660332 8.039463 8.891360

38 H 8.273277 6.896028 6.660332 8.039463 8.891360

39 H 8.401473 7.026553 6.495837 7.740537 8.778786

40 H 4.341070 5.432538 6.524673 6.378930 5.099630

41 H 4.341070 5.432538 6.524673 6.378930 5.099630

42 H 5.474107 6.399517 7.615385 7.659399 6.422930

43 H 8.264985 7.735877 8.831181 10.020771 9.687921

44 H 8.264985 7.735877 8.831181 10.020771 9.687921

45 H 9.120354 8.393029 9.355075 10.666001 10.508288

6 7 8 9 10

6 N 0.000000

7 C 1.340961 0.000000

8 N 2.413656 1.346306 0.000000

9 C 3.535739 2.228859 1.382929 0.000000

10 C 3.573843 2.294574 2.320037 1.484492 0.000000

11 C 2.490373 1.480995 2.293678 2.276267 1.357089

12 N 4.805543 5.337731 4.992421 6.256234 7.285903

13 C 6.842189 7.018221 6.256015 7.238355 8.541749

14 C 7.290243 7.217261 6.246681 7.012689 8.419114

15 C 6.272859 6.006624 4.926133 5.584686 7.018221

16 N 5.031997 4.926133 4.009877 4.923803 6.256015

17 C 5.359336 5.584686 4.923803 6.019430 7.238355

18 N 6.798113 6.272859 5.031997 5.359336 6.842189

19 N 5.029451 4.195811 2.861315 2.947189 4.431595

20 C 6.260921 5.509028 4.186240 4.241595 5.719517

21 C 7.291280 6.350069 5.005488 4.648704 6.028475

22 C 6.807453 5.701344 4.407756 3.722876 4.968131

23 C 5.363807 4.261273 2.962158 2.379725 3.752122

24 N 4.772760 3.509090 2.424997 1.319706 2.482272

25 Zn 3.399056 3.003312 2.004938 3.009715 4.270874

26 C 3.063289 4.403910 5.353134 6.580190 6.577538

27 H 4.605376 5.716157 6.046498 7.429259 7.994047

28 C 4.996802 3.762925 3.745217 2.624226 1.489282

29 H 2.844334 2.272668 3.321556 3.337756 2.194336

30 C 7.815894 8.174915 7.547315 8.612739 9.859606

31 H 8.345356 8.216007 7.185739 7.848833 9.289437

32 C 8.739111 7.829047 6.483221 6.120988 7.474314

33 H 7.511171 6.315483 5.098963 4.176469 5.205379

34 H 4.130591 5.470822 6.359397 7.621710 7.664593

35 H 3.061729 4.336899 5.388368 6.524828 6.379734

36 H 3.061729 4.336899 5.388368 6.524828 6.379734

37 H 5.591253 4.335314 4.145740 2.934089 2.141311

38 H 5.591253 4.335314 4.145740 2.934089 2.141311

39 H 5.240499 4.160722 4.454870 3.524625 2.142605

40 H 7.799779 8.260528 7.735884 8.859988 10.044253

41 H 7.799779 8.260528 7.735884 8.859988 10.044253

42 H 8.825782 9.109240 8.393079 9.377840 10.683636

43 H 9.077196 8.239756 6.904169 6.648751 8.027592

44 H 9.077196 8.239756 6.904169 6.648751 8.027592

45 H 9.384423 8.374478 7.044122 6.484468 7.730251

11 12 13 14 15

11 C 0.000000

12 N 6.816391 0.000000

13 C 8.419114 2.482272 0.000000

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16 N 6.246681 2.424997 2.320037 2.293678 1.346306

17 C 7.012689 1.319706 1.484492 2.276267 2.228859

18 N 7.290243 4.772760 3.573843 2.490373 1.340961

19 N 4.997335 4.989847 4.991781 4.398323 2.917381

20 C 6.334210 5.317396 4.659158 3.749680 2.372819

21 C 6.901330 6.803734 6.039077 4.994626 3.748147

22 C 5.995918 7.255493 6.918774 6.030126 4.648169

23 C 4.648663 6.265214 6.379876 5.738717 4.264015

24 N 3.541831 6.747639 7.285903 6.816391 5.337731

25 Zn 4.256902 3.373820 4.270874 4.256902 3.003312

26 C 5.351848 5.001977 7.474314 8.381455 7.829047

27 H 7.076323 2.858565 5.205379 6.378722 6.315483

28 C 2.577605 8.736218 9.859606 9.620159 8.174915

29 H 1.081305 7.518199 9.289437 9.471074 8.216007

30 C 9.620159 3.064781 1.489282 2.577605 3.762925

31 H 9.471074 4.568372 2.194336 1.081305 2.272668

32 C 8.381455 7.771369 6.577538 5.351848 4.403910

33 H 6.378722 8.313479 7.994047 7.076323 5.716157

34 H 6.443885 5.256080 7.730251 8.760183 8.374478

35 H 5.116230 5.595686 8.027592 8.872943 8.239756

36 H 5.116230 5.595686 8.027592 8.872943 8.239756

37 H 3.283961 9.072431 10.044253 9.718515 8.260528

38 H 3.283961 9.072431 10.044253 9.718515 8.260528

39 H 2.753482 9.379617 10.683636 10.531422 9.109240

40 H 9.718515 3.073728 2.141311 3.283961 4.335314

41 H 9.718515 3.073728 2.141311 3.283961 4.335314

42 H 10.531422 4.127735 2.142605 2.753482 4.160722

43 H 8.872943 7.753459 6.379734 5.116230 4.336899

44 H 8.872943 7.753459 6.379734 5.116230 4.336899

45 H 8.760183 8.784131 7.664593 6.443885 5.470822

16 17 18 19 20

16 N 0.000000

17 C 1.382929 0.000000

18 N 2.413656 3.535739 0.000000

19 N 2.815778 4.184139 2.426512 0.000000

20 C 2.907721 4.250357 1.359387 1.338225 0.000000

21 C 4.395095 5.730492 2.505319 2.296446 1.487619

22 C 4.968125 6.350432 3.582845 2.292233 2.283453

23 C 4.191143 5.545645 3.554891 1.389106 2.227611

24 N 4.992421 6.256234 4.805543 2.437809 3.525693

25 Zn 2.004938 3.009715 3.399056 2.009499 2.994987

26 C 6.483221 6.120988 8.739111 7.545775 8.584819

27 H 5.098963 4.176469 7.511171 7.177454 7.827784

28 C 7.547315 8.612739 7.815894 5.396164 6.576626

29 H 7.185739 7.848833 8.345356 6.073782 7.411445

30 C 3.745217 2.624226 4.996802 6.473534 6.134896

31 H 3.321556 3.337756 2.844334 5.080686 4.199809

32 C 5.353134 6.580190 3.063289 3.712962 2.624770

33 H 6.046498 7.429259 4.605376 3.328714 3.344503

34 H 7.044122 6.484468 9.384423 8.393029 9.355075

35 H 6.904169 6.648751 9.077196 7.735877 8.831181

36 H 6.904169 6.648751 9.077196 7.735877 8.831181

37 H 7.735884 8.859988 7.799779 5.432538 6.524673

38 H 7.735884 8.859988 7.799779 5.432538 6.524673

39 H 8.393079 9.377840 8.825782 6.399517 7.615385

40 H 4.145740 2.934089 5.591253 6.896028 6.660332

41 H 4.145740 2.934089 5.591253 6.896028 6.660332

42 H 4.454870 3.524625 5.240499 7.026553 6.495837

43 H 5.388368 6.524828 3.061729 4.110339 2.934729

44 H 5.388368 6.524828 3.061729 4.110339 2.934729

45 H 6.359397 7.621710 4.130591 4.433425 3.527673

21 22 23 24 25

21 C 0.000000

22 C 1.370627 0.000000

23 C 2.278853 1.445600 0.000000

24 N 3.578651 2.488807 1.346447 0.000000

25 Zn 4.262172 4.246824 3.024938 3.373820 0.000000

26 C 9.837291 9.592117 8.181833 7.771369 5.596813

27 H 9.273527 9.456208 8.233199 8.313479 5.221112

28 C 6.573340 5.331193 4.408061 3.064781 5.610217

29 H 7.976512 7.042810 5.716504 4.568372 5.226281

30 C 7.488156 8.402290 7.862478 8.736218 5.610217

31 H 5.228335 6.410763 6.344297 7.518199 5.226281

32 C 1.486122 2.590549 3.742558 5.001977 5.596813

33 H 2.203163 1.082205 2.243871 2.858565 5.221112

34 H 10.666001 10.508288 9.120354 8.784131 6.403984

35 H 10.020771 9.687921 8.264985 7.753459 5.859288

36 H 10.020771 9.687921 8.264985 7.753459 5.859288

37 H 6.378930 5.099630 4.341070 3.073728 5.873308

38 H 6.378930 5.099630 4.341070 3.073728 5.873308

39 H 7.659399 6.422930 5.474107 4.127735 6.412881

40 H 8.039463 8.891360 8.273277 9.072431 5.873308

41 H 8.039463 8.891360 8.273277 9.072431 5.873308

42 H 7.740537 8.778786 8.401473 9.379617 6.412881

43 H 2.139831 3.298139 4.318915 5.595686 5.859288

44 H 2.139831 3.298139 4.318915 5.595686 5.859288

45 H 2.142582 2.769282 4.140250 5.256080 6.403984

26 27 28 29 30

26 C 0.000000

27 H 2.998807 0.000000

28 C 7.928388 9.475251 0.000000

29 H 5.281154 7.402775 2.988331 0.000000

30 C 7.920755 5.262004 11.220433 10.423385 0.000000

31 H 9.454421 7.372039 10.423385 10.452562 2.988331

32 C 11.193626 10.400760 7.920755 9.454421 7.928388

33 H 10.400760 10.442223 5.262004 7.372039 9.475251

34 H 1.092049 2.759819 9.020307 6.355455 7.975284

35 H 1.097064 3.753471 7.663374 4.934906 8.537228

36 H 1.097064 3.753471 7.663374 4.934906 8.537228

37 H 8.542628 9.965493 1.096386 3.741353 11.434094

38 H 8.542628 9.965493 1.096386 3.741353 11.434094

39 H 7.979806 9.828969 1.091813 2.745075 12.000296

40 H 7.659219 4.919396 11.434094 10.470043 1.096386

41 H 7.659219 4.919396 11.434094 10.470043 1.096386

42 H 9.012293 6.337308 12.000296 11.372892 1.091813

43 H 11.406471 10.444806 8.537228 9.946720 7.663374

44 H 11.406471 10.444806 8.537228 9.946720 7.663374

45 H 11.978234 11.354534 7.975284 9.811128 9.020307

31 32 33 34 35

31 H 0.000000

32 C 5.281154 0.000000

33 H 7.402775 2.998807 0.000000

34 H 9.811128 11.978234 11.354534 0.000000

35 H 9.946720 11.406471 10.444806 1.775156 0.000000

36 H 9.946720 11.406471 10.444806 1.775156 1.757937

37 H 10.470043 7.659219 4.919396 9.628025 8.203441

38 H 10.470043 7.659219 4.919396 9.628025 8.389865

39 H 11.372892 9.012293 6.337308 9.064854 7.637445

40 H 3.741353 8.542628 9.965493 7.636403 8.201473

41 H 3.741353 8.542628 9.965493 7.636403 8.387941

42 H 2.745075 7.979806 9.828969 9.060934 9.621956

43 H 4.934906 1.097064 3.753471 12.146331 11.585969

44 H 4.934906 1.097064 3.753471 12.146331 11.718575

45 H 6.355455 1.092049 2.759819 12.807968 12.146331

36 37 38 39 40

36 H 0.000000

37 H 8.389865 0.000000

38 H 8.203441 1.759671 0.000000

39 H 7.637445 1.775043 1.775043 0.000000

40 H 8.387941 11.614067 11.746616 12.169257 0.000000

41 H 8.201473 11.746616 11.614067 12.169257 1.759671

42 H 9.621956 12.169257 12.169257 12.825762 1.775043

43 H 11.718575 8.201473 8.387941 9.621956 8.203441

44 H 11.585969 8.387941 8.201473 9.621956 8.389865

45 H 12.146331 7.636403 7.636403 9.060934 9.628025

41 42 43 44 45

41 H 0.000000

42 H 1.775043 0.000000

43 H 8.389865 7.637445 0.000000

44 H 8.203441 7.637445 1.757937 0.000000

45 H 9.628025 9.064854 1.775156 1.775156 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=3 Diff= 1.08D-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

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1 6 0 -2.819323 1.096206 0.000000

2 7 0 -2.009241 -0.032235 0.000000

3 6 0 -2.773256 -1.130928 0.000000

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5 6 0 -4.195989 0.655126 0.000000

6 7 0 -2.375771 -2.430905 0.000000

7 6 0 -1.086568 -2.799867 0.000000

8 7 0 0.000000 -2.004938 0.000000

9 6 0 1.142239 -2.784542 0.000000

10 6 0 0.724347 -4.209001 0.000000

11 6 0 -0.632742 -4.209614 0.000000

12 7 0 -2.396657 2.374593 0.000000

13 6 0 -0.724347 4.209001 0.000000

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16 7 0 0.000000 2.004938 0.000000

17 6 0 -1.142239 2.784542 0.000000

18 7 0 2.375771 2.430905 0.000000

19 7 0 2.009241 0.032235 0.000000

20 6 0 2.773256 1.130928 0.000000

21 6 0 4.201688 0.715489 0.000000

22 6 0 4.195989 -0.655126 0.000000

23 6 0 2.819323 -1.096206 0.000000

24 7 0 2.396657 -2.374593 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -5.342513 -1.667895 0.000000

27 1 0 -5.052321 1.316838 0.000000

28 6 0 1.677047 -5.353695 0.000000

29 1 0 -1.297089 -5.062763 0.000000

30 6 0 -1.677047 5.353695 0.000000

31 1 0 1.297089 5.062763 0.000000

32 6 0 5.342513 1.667895 0.000000

33 1 0 5.052321 -1.316838 0.000000

34 1 0 -6.300903 -1.144390 0.000000

35 1 0 -5.306648 -2.323393 0.878969

36 1 0 -5.306648 -2.323393 -0.878969

37 1 0 2.330304 -5.318959 0.879836

38 1 0 2.330304 -5.318959 -0.879836

39 1 0 1.148709 -6.309161 0.000000

40 1 0 -2.330304 5.318959 0.879836

41 1 0 -2.330304 5.318959 -0.879836

42 1 0 -1.148709 6.309161 0.000000

43 1 0 5.306648 2.323393 0.878969

44 1 0 5.306648 2.323393 -0.878969

45 1 0 6.300903 1.144390 0.000000

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

Rotational constants (GHZ): 0.1826968 0.1818880 0.0913512

Leave Link 202 at Tue Sep 17 13:58:24 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 101 beta electrons

nuclear repulsion energy 2760.7570120958 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= -0.1142256563 Hartrees.

Nuclear repulsion after empirical dispersion term = 2760.6427864395 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 = 3500

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.13D-07

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 136

GePol: Fraction of low-weight points (<1% of avg) = 3.89%

GePol: Cavity surface area = 382.480 Ang\*\*2

GePol: Cavity volume = 379.838 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0107377618 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2760.6320486777 Hartrees.

Leave Link 301 at Tue Sep 17 13:58:24 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= 15333 LenP2D= 41260.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.86D-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 13:58:25 2019, MaxMem= 2415919104 cpu: 12.5

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 13:58:25 2019, MaxMem= 2415919104 cpu: 1.3

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= 0.000000 0.000000 -0.000000

Rot= 1.000000 -0.000000 -0.000000 -0.000419 Ang= -0.05 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 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0391 S= 1.0130

Leave Link 401 at Tue Sep 17 13:58:26 2019, MaxMem= 2415919104 cpu: 21.1

(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= 36750000.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.99D-15 for 3497.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.37D-15 for 2021 1848.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.22D-15 for 3497.

Iteration 1 A^-1\*A deviation from orthogonality is 1.83D-11 for 1983 1973.

E= -1275.84074974928

DIIS: error= 6.03D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.84074974928 IErMin= 1 ErrMin= 6.03D-04

ErrMax= 6.03D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.30D-04 BMatP= 4.30D-04

IDIUse=3 WtCom= 9.94D-01 WtEn= 6.03D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.301 Goal= None Shift= 0.000

Gap= 0.395 Goal= None Shift= 0.000

RMSDP=4.29D-05 MaxDP=1.34D-03 OVMax= 2.64D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.29D-05 CP: 1.00D+00

E= -1275.84095104092 Delta-E= -0.000201291637 Rises=F Damp=F

DIIS: error= 3.37D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84095104092 IErMin= 2 ErrMin= 3.37D-04

ErrMax= 3.37D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.90D-05 BMatP= 4.30D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.37D-03

Coeff-Com: 0.792D-01 0.921D+00

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

Coeff: 0.789D-01 0.921D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.085 Goal= None Shift= 0.000

RMSDP=2.14D-05 MaxDP=7.80D-04 DE=-2.01D-04 OVMax= 1.61D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.42D-05 CP: 1.00D+00 1.37D+00

E= -1275.84098857381 Delta-E= -0.000037532895 Rises=F Damp=F

DIIS: error= 3.22D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1275.84098857381 IErMin= 3 ErrMin= 3.22D-04

ErrMax= 3.22D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.05D-05 BMatP= 3.90D-05

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.22D-03

Coeff-Com: -0.519D-02 0.387D+00 0.618D+00

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

Coeff: -0.517D-02 0.386D+00 0.619D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.085 Goal= None Shift= 0.000

RMSDP=1.38D-05 MaxDP=6.01D-04 DE=-3.75D-05 OVMax= 1.06D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 8.20D-06 CP: 1.00D+00 1.59D+00 1.40D+00

E= -1275.84100785182 Delta-E= -0.000019278012 Rises=F Damp=F

DIIS: error= 2.26D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84100785182 IErMin= 4 ErrMin= 2.26D-04

ErrMax= 2.26D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.46D-05 BMatP= 2.05D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.26D-03

Coeff-Com: -0.891D-02 0.241D-01 0.451D+00 0.534D+00

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

Coeff: -0.889D-02 0.240D-01 0.450D+00 0.535D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.08D-05 MaxDP=4.07D-04 DE=-1.93D-05 OVMax= 8.40D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.33D-06 CP: 1.00D+00 1.78D+00 1.89D+00 1.17D+00

E= -1275.84102255396 Delta-E= -0.000014702139 Rises=F Damp=F

DIIS: error= 1.96D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84102255396 IErMin= 5 ErrMin= 1.96D-04

ErrMax= 1.96D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.60D-06 BMatP= 1.46D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.96D-03

Coeff-Com: 0.594D-02-0.208D+00 0.101D-01-0.111D-01 0.120D+01

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

Coeff: 0.592D-02-0.208D+00 0.101D-01-0.111D-01 0.120D+01

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.92D-05 MaxDP=7.93D-04 DE=-1.47D-05 OVMax= 1.54D-02

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.75D-06 CP: 1.00D+00 2.10D+00 2.71D+00 1.85D+00 1.64D+00

E= -1275.84103976126 Delta-E= -0.000017207302 Rises=F Damp=F

DIIS: error= 1.24D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84103976126 IErMin= 6 ErrMin= 1.24D-04

ErrMax= 1.24D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.06D-06 BMatP= 3.60D-06

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.24D-03

Coeff-Com: 0.150D-01-0.221D+00-0.338D+00-0.673D+00 0.105D+01 0.117D+01

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

Coeff: 0.150D-01-0.220D+00-0.337D+00-0.672D+00 0.105D+01 0.117D+01

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=2.84D-05 MaxDP=1.14D-03 DE=-1.72D-05 OVMax= 2.28D-02

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.36D-05 CP: 1.00D+00 2.58D+00 3.00D+00 2.77D+00 3.00D+00

CP: 2.02D+00

E= -1275.84105315978 Delta-E= -0.000013398519 Rises=F Damp=F

DIIS: error= 4.04D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84105315978 IErMin= 7 ErrMin= 4.04D-05

ErrMax= 4.04D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.17D-07 BMatP= 3.06D-06

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

Coeff-Com: 0.583D-02-0.415D-01-0.129D+00-0.343D+00 0.240D+00 0.514D+00

Coeff-Com: 0.753D+00

Coeff: 0.583D-02-0.415D-01-0.129D+00-0.343D+00 0.240D+00 0.514D+00

Coeff: 0.753D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=6.44D-06 MaxDP=2.61D-04 DE=-1.34D-05 OVMax= 5.12D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.14D-06 CP: 1.00D+00 2.69D+00 3.00D+00 3.00D+00 3.00D+00

CP: 2.59D+00 1.29D+00

E= -1275.84105424846 Delta-E= -0.000001088678 Rises=F Damp=F

DIIS: error= 3.27D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84105424846 IErMin= 8 ErrMin= 3.27D-05

ErrMax= 3.27D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.37D-07 BMatP= 6.17D-07

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

Coeff-Com: -0.468D-02 0.104D+00 0.120D+00 0.141D+00-0.409D+00-0.338D+00

Coeff-Com: 0.534D+00 0.853D+00

Coeff: -0.468D-02 0.104D+00 0.120D+00 0.141D+00-0.409D+00-0.338D+00

Coeff: 0.534D+00 0.853D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=2.80D-06 MaxDP=1.15D-04 DE=-1.09D-06 OVMax= 2.02D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.15D-06 CP: 1.00D+00 2.73D+00 3.00D+00 3.00D+00 3.00D+00

CP: 2.94D+00 1.41D+00 1.40D+00

E= -1275.84105462666 Delta-E= -0.000000378201 Rises=F Damp=F

DIIS: error= 1.18D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84105462666 IErMin= 9 ErrMin= 1.18D-05

ErrMax= 1.18D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.90D-08 BMatP= 3.37D-07

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

Coeff-Com: -0.253D-02 0.377D-01 0.624D-01 0.127D+00-0.181D+00-0.208D+00

Coeff-Com: -0.303D-01 0.328D+00 0.867D+00

Coeff: -0.253D-02 0.377D-01 0.624D-01 0.127D+00-0.181D+00-0.208D+00

Coeff: -0.303D-01 0.328D+00 0.867D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=7.96D-07 MaxDP=3.68D-05 DE=-3.78D-07 OVMax= 4.66D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 3.64D-07 CP: 1.00D+00 2.73D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.44D+00 1.65D+00 1.27D+00

E= -1275.84105468784 Delta-E= -0.000000061180 Rises=F Damp=F

DIIS: error= 5.06D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84105468784 IErMin=10 ErrMin= 5.06D-06

ErrMax= 5.06D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.58D-08 BMatP= 5.90D-08

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

Coeff-Com: -0.543D-03 0.140D-03 0.137D-01 0.559D-01-0.289D-01-0.559D-01

Coeff-Com: -0.141D+00 0.197D-01 0.503D+00 0.634D+00

Coeff: -0.543D-03 0.140D-03 0.137D-01 0.559D-01-0.289D-01-0.559D-01

Coeff: -0.141D+00 0.197D-01 0.503D+00 0.634D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=2.61D-07 MaxDP=1.49D-05 DE=-6.12D-08 OVMax= 9.55D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.83D-07 CP: 1.00D+00 2.74D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.45D+00 1.71D+00 1.38D+00 1.22D+00

E= -1275.84105470400 Delta-E= -0.000000016154 Rises=F Damp=F

DIIS: error= 2.74D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84105470400 IErMin=11 ErrMin= 2.74D-06

ErrMax= 2.74D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.47D-09 BMatP= 2.58D-08

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

Coeff-Com: 0.617D-03-0.121D-01-0.161D-01-0.218D-01 0.405D-01 0.483D-01

Coeff-Com: -0.279D-01-0.803D-01-0.936D-01 0.234D+00 0.928D+00

Coeff: 0.617D-03-0.121D-01-0.161D-01-0.218D-01 0.405D-01 0.483D-01

Coeff: -0.279D-01-0.803D-01-0.936D-01 0.234D+00 0.928D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=3.99D-07 MaxDP=1.41D-05 DE=-1.62D-08 OVMax= 2.92D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.17D-07 CP: 1.00D+00 2.74D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.46D+00 1.76D+00 1.48D+00 1.52D+00

CP: 1.17D+00

E= -1275.84105471131 Delta-E= -0.000000007311 Rises=F Damp=F

DIIS: error= 1.80D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84105471131 IErMin=12 ErrMin= 1.80D-06

ErrMax= 1.80D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.79D-09 BMatP= 4.47D-09

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

Coeff-Com: 0.458D-03-0.632D-02-0.114D-01-0.263D-01 0.303D-01 0.384D-01

Coeff-Com: 0.173D-01-0.506D-01-0.174D+00-0.616D-01 0.503D+00 0.741D+00

Coeff: 0.458D-03-0.632D-02-0.114D-01-0.263D-01 0.303D-01 0.384D-01

Coeff: 0.173D-01-0.506D-01-0.174D+00-0.616D-01 0.503D+00 0.741D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.57D-07 MaxDP=7.77D-06 DE=-7.31D-09 OVMax= 9.88D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 4.15D-08 CP: 1.00D+00 2.74D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.47D+00 1.79D+00 1.52D+00 1.67D+00

CP: 1.41D+00 1.25D+00

E= -1275.84105471331 Delta-E= -0.000000002006 Rises=F Damp=F

DIIS: error= 6.90D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84105471331 IErMin=13 ErrMin= 6.90D-07

ErrMax= 6.90D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.10D-10 BMatP= 1.79D-09

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

Coeff-Com: -0.100D-03 0.309D-02 0.341D-02-0.122D-02-0.480D-02-0.793D-02

Coeff-Com: 0.161D-01 0.105D-01-0.369D-01-0.148D+00-0.113D+00 0.400D+00

Coeff-Com: 0.879D+00

Coeff: -0.100D-03 0.309D-02 0.341D-02-0.122D-02-0.480D-02-0.793D-02

Coeff: 0.161D-01 0.105D-01-0.369D-01-0.148D+00-0.113D+00 0.400D+00

Coeff: 0.879D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=8.07D-08 MaxDP=5.00D-06 DE=-2.01D-09 OVMax= 3.55D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 2.98D-08 CP: 1.00D+00 2.74D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.47D+00 1.81D+00 1.55D+00 1.76D+00

CP: 1.61D+00 1.42D+00 1.16D+00

E= -1275.84105471387 Delta-E= -0.000000000558 Rises=F Damp=F

DIIS: error= 2.54D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84105471387 IErMin=14 ErrMin= 2.54D-07

ErrMax= 2.54D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.89D-11 BMatP= 5.10D-10

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

Coeff-Com: -0.830D-04 0.193D-02 0.239D-02 0.134D-02-0.504D-02-0.667D-02

Coeff-Com: 0.626D-02 0.108D-01-0.934D-03-0.635D-01-0.107D+00 0.103D+00

Coeff-Com: 0.432D+00 0.625D+00

Coeff: -0.830D-04 0.193D-02 0.239D-02 0.134D-02-0.504D-02-0.667D-02

Coeff: 0.626D-02 0.108D-01-0.934D-03-0.635D-01-0.107D+00 0.103D+00

Coeff: 0.432D+00 0.625D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=3.91D-08 MaxDP=1.61D-06 DE=-5.58D-10 OVMax= 2.90D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 8.60D-09 CP: 1.00D+00 2.74D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.47D+00 1.82D+00 1.56D+00 1.78D+00

CP: 1.63D+00 1.49D+00 1.28D+00 9.72D-01

E= -1275.84105471395 Delta-E= -0.000000000075 Rises=F Damp=F

DIIS: error= 1.26D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.84105471395 IErMin=15 ErrMin= 1.26D-07

ErrMax= 1.26D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.46D-11 BMatP= 8.89D-11

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

Coeff-Com: -0.167D-04 0.358D-04 0.377D-03 0.182D-02-0.158D-02-0.136D-02

Coeff-Com: -0.302D-02 0.341D-02 0.147D-01 0.205D-01-0.263D-01-0.102D+00

Coeff-Com: -0.771D-01 0.352D+00 0.818D+00

Coeff: -0.167D-04 0.358D-04 0.377D-03 0.182D-02-0.158D-02-0.136D-02

Coeff: -0.302D-02 0.341D-02 0.147D-01 0.205D-01-0.263D-01-0.102D+00

Coeff: -0.771D-01 0.352D+00 0.818D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.04D-08 MaxDP=7.70D-07 DE=-7.50D-11 OVMax= 4.72D-06

Cycle 16 Pass 1 IDiag 1:

RMSU= 4.71D-09 CP: 1.00D+00 2.74D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.47D+00 1.82D+00 1.56D+00 1.79D+00

CP: 1.65D+00 1.52D+00 1.37D+00 1.17D+00 1.10D+00

E= -1275.84105471396 Delta-E= -0.000000000016 Rises=F Damp=F

DIIS: error= 6.47D-08 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1275.84105471396 IErMin=16 ErrMin= 6.47D-08

ErrMax= 6.47D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.10D-12 BMatP= 2.46D-11

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

Coeff-Com: -0.344D-05-0.124D-03 0.274D-04 0.100D-02-0.563D-03-0.275D-03

Coeff-Com: -0.229D-02 0.105D-02 0.837D-02 0.174D-01-0.197D-02-0.624D-01

Coeff-Com: -0.822D-01 0.834D-01 0.386D+00 0.652D+00

Coeff: -0.344D-05-0.124D-03 0.274D-04 0.100D-02-0.563D-03-0.275D-03

Coeff: -0.229D-02 0.105D-02 0.837D-02 0.174D-01-0.197D-02-0.624D-01

Coeff: -0.822D-01 0.834D-01 0.386D+00 0.652D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=3.84D-09 MaxDP=2.32D-07 DE=-1.59D-11 OVMax= 2.04D-06

Error on total polarization charges = 0.06475

SCF Done: E(UB3LYP) = -1275.84105471 A.U. after 16 cycles

NFock= 16 Conv=0.38D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0342 S= 1.0113

<L.S>= 0.000000000000E+00

KE= 1.320757706164D+03 PE=-8.573201484320D+03 EE= 3.215970674764D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.74

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0342, after 2.0007

Leave Link 502 at Tue Sep 17 13:59:58 2019, MaxMem= 2415919104 cpu: 1606.0

(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= 15333 LenP2D= 41260.

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 = 246

Leave Link 701 at Tue Sep 17 14:00:02 2019, MaxMem= 2415919104 cpu: 72.7

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 14:00:02 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 14:00:12 2019, MaxMem= 2415919104 cpu: 192.2

(Enter /home/blab/g09/l716.exe)

Dipole =-1.59872116D-13 1.55875313D-13 0.00000000D+00

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.008115442 -0.001743799 -0.000000000

2 7 -0.004924008 0.001734669 -0.000000000

3 6 -0.000990142 -0.004922234 0.000000000

4 6 0.001674119 0.003798515 0.000000000

5 6 -0.001620521 -0.000472755 0.000000000

6 7 0.003352662 0.003100194 0.000000000

7 6 -0.002149846 -0.006930460 -0.000000000

8 7 0.001877287 0.004954706 0.000000000

9 6 -0.005624611 0.001530595 0.000000000

10 6 0.002138013 -0.003253538 0.000000000

11 6 0.001066714 0.002973420 0.000000000

12 7 -0.006194127 0.003030834 0.000000000

13 6 -0.002138013 0.003253538 -0.000000000

14 6 -0.001066714 -0.002973420 0.000000000

15 6 0.002149846 0.006930460 0.000000000

16 7 -0.001877287 -0.004954706 -0.000000000

17 6 0.005624611 -0.001530595 0.000000000

18 7 -0.003352662 -0.003100194 -0.000000000

19 7 0.004924008 -0.001734669 -0.000000000

20 6 0.000990142 0.004922234 0.000000000

21 6 -0.001674119 -0.003798515 -0.000000000

22 6 0.001620521 0.000472755 0.000000000

23 6 -0.008115442 0.001743799 0.000000000

24 7 0.006194127 -0.003030834 0.000000000

25 30 0.000000000 -0.000000000 0.000000000

26 6 0.000373360 -0.000645748 0.000000000

27 1 0.000644220 0.000061402 0.000000000

28 6 -0.000255144 0.000074985 -0.000000000

29 1 0.000025905 0.000175887 -0.000000000

30 6 0.000255144 -0.000074985 -0.000000000

31 1 -0.000025905 -0.000175887 0.000000000

32 6 -0.000373360 0.000645748 -0.000000000

33 1 -0.000644220 -0.000061402 -0.000000000

34 1 0.000359438 0.000293954 0.000000000

35 1 -0.000468746 0.000006051 -0.001042096

36 1 -0.000468746 0.000006051 0.001042096

37 1 -0.000282138 -0.000462712 -0.001115856

38 1 -0.000282138 -0.000462712 0.001115856

39 1 -0.000362283 0.000399492 -0.000000000

40 1 0.000282138 0.000462712 -0.001115856

41 1 0.000282138 0.000462712 0.001115856

42 1 0.000362283 -0.000399492 -0.000000000

43 1 0.000468746 -0.000006051 -0.001042096

44 1 0.000468746 -0.000006051 0.001042096

45 1 -0.000359438 -0.000293954 0.000000000

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

Cartesian Forces: Max 0.008115442 RMS 0.002299645

Leave Link 716 at Tue Sep 17 14:00:13 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 0.004588003 RMS 0.000881836

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= -2.24D-04 DEPred=-1.16D-04 R= 1.94D+00

TightC=F SS= 1.41D+00 RLast= 3.44D-02 DXNew= 5.0454D-01 1.0312D-01

Trust test= 1.94D+00 RLast= 3.44D-02 DXMaxT set to 3.00D-01

ITU= 1 1 1 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01341

Eigenvalues --- 0.01343 0.01343 0.01343 0.01371 0.01604

Eigenvalues --- 0.01622 0.01635 0.01637 0.01775 0.01791

Eigenvalues --- 0.01814 0.01818 0.01890 0.01906 0.01940

Eigenvalues --- 0.01947 0.01998 0.01999 0.02042 0.02050

Eigenvalues --- 0.02070 0.02088 0.02103 0.02111 0.02114

Eigenvalues --- 0.02205 0.02311 0.02319 0.02351 0.02374

Eigenvalues --- 0.07188 0.07188 0.07225 0.07225 0.07355

Eigenvalues --- 0.07363 0.07376 0.07445 0.14484 0.14512

Eigenvalues --- 0.15077 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 0.16014 0.16072

Eigenvalues --- 0.16142 0.16734 0.17893 0.18476 0.22066

Eigenvalues --- 0.22097 0.23841 0.23853 0.23894 0.24203

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25001 0.25026 0.25335

Eigenvalues --- 0.25740 0.30073 0.31030 0.33194 0.33198

Eigenvalues --- 0.33282 0.33282 0.33335 0.33372 0.33689

Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33735 0.34380 0.34437 0.34437

Eigenvalues --- 0.34438 0.35006 0.35555 0.35563 0.35598

Eigenvalues --- 0.35682 0.35682 0.35747 0.38006 0.39131

Eigenvalues --- 0.40676 0.40990 0.41684 0.41782 0.47804

Eigenvalues --- 0.48520 0.48932 0.49020 0.50676 0.51354

Eigenvalues --- 0.51365 0.51496 0.53985 0.54041 0.54364

Eigenvalues --- 0.56301 0.56356 0.56358 1.43486

Cosine: 0.488 < 0.840

Cut down GDIIS temporarily because of the cosine check. E 7

DIIS coeff's: 7.84271 -6.84271

Cosine: 1.000 > 0.970

Length: 1.000

GDIIS step was calculated using 2 of the last 6 vectors.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.590

Iteration 1 RMS(Cart)= 0.02007058 RMS(Int)= 0.00026825

Iteration 2 RMS(Cart)= 0.00030607 RMS(Int)= 0.00007828

Iteration 3 RMS(Cart)= 0.00000011 RMS(Int)= 0.00007828

ITry= 1 IFail=0 DXMaxC= 7.86D-02 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 3.92D-09 for atom 38.

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

(Linear) (Quad) (Total)

R1 2.62503 -0.00296 -0.00365 -0.01321 -0.01658 2.60845

R2 2.73179 -0.00031 -0.02619 -0.02797 -0.05426 2.67753

R3 2.54442 0.00459 0.03010 0.04140 0.07154 2.61596

R4 2.52888 0.00246 0.00195 0.00846 0.01071 2.53959

R5 3.79740 -0.00024 0.00926 0.00999 0.01955 3.81695

R6 2.81119 -0.00289 -0.02686 -0.03758 -0.06444 2.74675

R7 2.56887 0.00131 0.02884 0.03266 0.06153 2.63040

R8 2.59011 -0.00013 0.02628 0.02921 0.05533 2.64544

R9 2.80836 0.00026 0.00369 0.00481 0.00850 2.81687

R10 2.04507 -0.00059 0.00277 0.00225 0.00502 2.05010

R11 2.53405 -0.00337 -0.03547 -0.04510 -0.08068 2.45337

R12 2.54415 0.00339 0.00748 0.01578 0.02308 2.56723

R13 2.79867 0.00020 0.01765 0.01887 0.03651 2.83519

R14 2.61336 -0.00221 -0.00082 -0.00837 -0.00939 2.60396

R15 3.78878 -0.00028 -0.00144 -0.00334 -0.00496 3.78382

R16 2.80528 0.00221 0.02064 0.02936 0.05001 2.85530

R17 2.49388 -0.00099 -0.03206 -0.03519 -0.06737 2.42652

R18 2.56453 -0.00254 -0.00770 -0.01225 -0.01993 2.54460

R19 2.81434 -0.00126 0.00416 0.00254 0.00670 2.82103

R20 2.04337 -0.00014 0.00114 0.00101 0.00216 2.04553

R21 2.49388 -0.00099 -0.03206 -0.03519 -0.06737 2.42652

R22 2.56453 -0.00254 -0.00770 -0.01225 -0.01993 2.54460

R23 2.80528 0.00221 0.02064 0.02936 0.05001 2.85530

R24 2.81434 -0.00126 0.00416 0.00254 0.00670 2.82103

R25 2.79867 0.00020 0.01765 0.01887 0.03651 2.83519

R26 2.04337 -0.00014 0.00114 0.00101 0.00216 2.04553

R27 2.54415 0.00339 0.00748 0.01578 0.02308 2.56723

R28 2.53405 -0.00337 -0.03547 -0.04510 -0.08068 2.45337

R29 2.61336 -0.00221 -0.00082 -0.00837 -0.00939 2.60396

R30 3.78878 -0.00028 -0.00144 -0.00334 -0.00496 3.78382

R31 2.56887 0.00131 0.02884 0.03266 0.06153 2.63040

R32 2.52888 0.00246 0.00195 0.00846 0.01071 2.53959

R33 2.62503 -0.00296 -0.00365 -0.01321 -0.01658 2.60845

R34 3.79740 -0.00024 0.00926 0.00999 0.01955 3.81695

R35 2.81119 -0.00289 -0.02686 -0.03758 -0.06444 2.74675

R36 2.59011 -0.00013 0.02628 0.02921 0.05533 2.64544

R37 2.80836 0.00026 0.00369 0.00481 0.00850 2.81687

R38 2.73179 -0.00031 -0.02619 -0.02797 -0.05426 2.67753

R39 2.04507 -0.00059 0.00277 0.00225 0.00502 2.05010

R40 2.54442 0.00459 0.03010 0.04140 0.07154 2.61596

R41 2.06367 -0.00046 0.00297 0.00261 0.00557 2.06925

R42 2.07315 -0.00110 0.00607 0.00499 0.01106 2.08421

R43 2.07315 -0.00110 0.00607 0.00499 0.01106 2.08421

R44 2.07187 -0.00121 0.00598 0.00502 0.01100 2.08287

R45 2.07187 -0.00121 0.00598 0.00502 0.01100 2.08287

R46 2.06323 -0.00054 0.00279 0.00227 0.00505 2.06828

R47 2.07187 -0.00121 0.00598 0.00502 0.01100 2.08287

R48 2.07187 -0.00121 0.00598 0.00502 0.01100 2.08287

R49 2.06323 -0.00054 0.00279 0.00227 0.00505 2.06828

R50 2.07315 -0.00110 0.00607 0.00499 0.01106 2.08421

R51 2.07315 -0.00110 0.00607 0.00499 0.01106 2.08421

R52 2.06367 -0.00046 0.00297 0.00261 0.00557 2.06925

A1 1.88336 0.00040 0.00220 0.00455 0.00674 1.89009

A2 2.19966 0.00048 -0.01189 -0.01071 -0.02234 2.17732

A3 2.20017 -0.00087 0.00968 0.00615 0.01560 2.21577

A4 1.91135 0.00000 -0.00393 -0.00507 -0.00904 1.90231

A5 2.17738 0.00048 -0.00750 -0.00517 -0.01261 2.16477

A6 2.19446 -0.00048 0.01143 0.01024 0.02165 2.21611

A7 1.89539 -0.00063 0.00838 0.00854 0.01708 1.91247

A8 2.23724 -0.00019 -0.01860 -0.02249 -0.04095 2.19628

A9 2.15056 0.00082 0.01022 0.01395 0.02388 2.17444

A10 1.84967 0.00069 -0.00913 -0.00827 -0.01741 1.83226

A11 2.16294 0.00027 0.01250 0.01583 0.02833 2.19127

A12 2.27058 -0.00096 -0.00337 -0.00756 -0.01093 2.25965

A13 1.88502 -0.00046 0.00248 0.00024 0.00263 1.88765

A14 2.17364 0.00051 0.00158 0.00442 0.00605 2.17969

A15 2.22453 -0.00004 -0.00406 -0.00467 -0.00868 2.21585

A16 2.14628 0.00029 0.00708 0.01161 0.01869 2.16496

A17 2.23123 0.00044 0.00275 0.00338 0.00599 2.23722

A18 2.16098 0.00044 -0.00396 -0.00244 -0.00625 2.15473

A19 1.89097 -0.00089 0.00120 -0.00093 0.00026 1.89123

A20 1.91108 0.00002 -0.00018 0.00087 0.00078 1.91185

A21 2.20241 -0.00052 0.00581 0.00320 0.00902 2.21144

A22 2.16970 0.00050 -0.00562 -0.00408 -0.00980 2.15990

A23 1.88433 -0.00018 -0.00159 -0.00192 -0.00348 1.88086

A24 2.22683 0.00128 0.00025 0.00522 0.00527 2.23210

A25 2.17202 -0.00110 0.00134 -0.00330 -0.00179 2.17023

A26 1.85661 0.00044 0.00330 0.00329 0.00654 1.86315

A27 2.16212 -0.00021 -0.00681 -0.00777 -0.01456 2.14756

A28 2.26446 -0.00023 0.00351 0.00448 0.00802 2.27248

A29 1.88179 0.00061 -0.00273 -0.00131 -0.00410 1.87769

A30 2.16853 -0.00019 -0.00234 -0.00296 -0.00527 2.16326

A31 2.23287 -0.00041 0.00507 0.00427 0.00937 2.24224

A32 2.20597 -0.00227 0.01628 0.00880 0.02508 2.23105

A33 1.85661 0.00044 0.00330 0.00329 0.00654 1.86315

A34 2.26446 -0.00023 0.00351 0.00448 0.00802 2.27248

A35 2.16212 -0.00021 -0.00681 -0.00777 -0.01456 2.14756

A36 1.88179 0.00061 -0.00273 -0.00131 -0.00410 1.87769

A37 2.23287 -0.00041 0.00507 0.00427 0.00937 2.24224

A38 2.16853 -0.00019 -0.00234 -0.00296 -0.00527 2.16326

A39 1.89097 -0.00089 0.00120 -0.00093 0.00026 1.89123

A40 2.16098 0.00044 -0.00396 -0.00244 -0.00625 2.15473

A41 2.23123 0.00044 0.00275 0.00338 0.00599 2.23722

A42 1.91108 0.00002 -0.00018 0.00087 0.00078 1.91185

A43 2.20241 -0.00052 0.00581 0.00320 0.00902 2.21144

A44 2.16970 0.00050 -0.00562 -0.00408 -0.00980 2.15990

A45 2.17202 -0.00110 0.00134 -0.00330 -0.00179 2.17023

A46 2.22683 0.00128 0.00025 0.00522 0.00527 2.23210

A47 1.88433 -0.00018 -0.00159 -0.00192 -0.00348 1.88086

A48 2.14628 0.00029 0.00708 0.01161 0.01869 2.16496

A49 1.91135 0.00000 -0.00393 -0.00507 -0.00904 1.90231

A50 2.19446 -0.00048 0.01143 0.01024 0.02165 2.21611

A51 2.17738 0.00048 -0.00750 -0.00517 -0.01261 2.16477

A52 2.23724 -0.00019 -0.01860 -0.02249 -0.04095 2.19628

A53 2.15056 0.00082 0.01022 0.01395 0.02388 2.17444

A54 1.89539 -0.00063 0.00838 0.00854 0.01708 1.91247

A55 1.84967 0.00069 -0.00913 -0.00827 -0.01741 1.83226

A56 2.16294 0.00027 0.01250 0.01583 0.02833 2.19127

A57 2.27058 -0.00096 -0.00337 -0.00756 -0.01093 2.25965

A58 1.88502 -0.00046 0.00248 0.00024 0.00263 1.88765

A59 2.22453 -0.00004 -0.00406 -0.00467 -0.00868 2.21585

A60 2.17364 0.00051 0.00158 0.00442 0.00605 2.17969

A61 1.88336 0.00040 0.00220 0.00455 0.00674 1.89009

A62 2.19966 0.00048 -0.01189 -0.01071 -0.02234 2.17732

A63 2.20017 -0.00087 0.00968 0.00615 0.01560 2.21577

A64 2.20597 -0.00227 0.01628 0.00880 0.02508 2.23105

A65 1.55475 0.00046 -0.00848 -0.00593 -0.01440 1.54036

A66 1.58684 -0.00046 0.00848 0.00593 0.01440 1.60123

A67 1.58684 -0.00046 0.00848 0.00593 0.01440 1.60123

A68 1.55475 0.00046 -0.00848 -0.00593 -0.01440 1.54036

A69 1.94602 -0.00010 -0.00303 -0.00418 -0.00724 1.93877

A70 1.93673 0.00031 -0.00023 0.00093 0.00066 1.93739

A71 1.93673 0.00031 -0.00023 0.00093 0.00066 1.93739

A72 1.89138 -0.00009 -0.00277 -0.00319 -0.00599 1.88539

A73 1.89138 -0.00009 -0.00277 -0.00319 -0.00599 1.88539

A74 1.85860 -0.00037 0.00948 0.00912 0.01856 1.87715

A75 1.93564 -0.00000 -0.00391 -0.00413 -0.00806 1.92758

A76 1.93564 -0.00000 -0.00391 -0.00413 -0.00806 1.92758

A77 1.94236 0.00003 -0.00346 -0.00319 -0.00671 1.93565

A78 1.86290 -0.00021 0.01025 0.00882 0.01906 1.88197

A79 1.89236 0.00009 0.00089 0.00167 0.00251 1.89487

A80 1.89236 0.00009 0.00089 0.00167 0.00251 1.89487

A81 1.93564 -0.00000 -0.00391 -0.00413 -0.00806 1.92758

A82 1.93564 -0.00000 -0.00391 -0.00413 -0.00806 1.92758

A83 1.94236 0.00003 -0.00346 -0.00319 -0.00671 1.93565

A84 1.86290 -0.00021 0.01025 0.00882 0.01906 1.88197

A85 1.89236 0.00009 0.00089 0.00167 0.00251 1.89487

A86 1.89236 0.00009 0.00089 0.00167 0.00251 1.89487

A87 1.93673 0.00031 -0.00023 0.00093 0.00066 1.93739

A88 1.93673 0.00031 -0.00023 0.00093 0.00066 1.93739

A89 1.94602 -0.00010 -0.00303 -0.00418 -0.00724 1.93877

A90 1.85860 -0.00037 0.00948 0.00912 0.01856 1.87715

A91 1.89138 -0.00009 -0.00277 -0.00319 -0.00599 1.88539

A92 1.89138 -0.00009 -0.00277 -0.00319 -0.00599 1.88539

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

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D19 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

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 1.03138 -0.00003 0.00576 0.00628 0.01205 1.04343

D31 -1.03138 0.00003 -0.00576 -0.00628 -0.01205 -1.04343

D32 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D33 -2.11021 -0.00003 0.00576 0.00628 0.01205 -2.09816

D34 2.11021 0.00003 -0.00576 -0.00628 -0.01205 2.09816

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

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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 1.03337 -0.00013 0.00389 0.00285 0.00672 1.04009

D64 -1.03337 0.00013 -0.00389 -0.00285 -0.00672 -1.04009

D65 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D66 -2.10822 -0.00013 0.00389 0.00285 0.00672 -2.10150

D67 2.10822 0.00013 -0.00389 -0.00285 -0.00672 2.10150

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 -2.10822 -0.00013 0.00389 0.00285 0.00672 -2.10150

D80 2.10822 0.00013 -0.00389 -0.00285 -0.00672 2.10150

D81 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D82 1.03337 -0.00013 0.00389 0.00285 0.00672 1.04009

D83 -1.03337 0.00013 -0.00389 -0.00285 -0.00672 -1.04009

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

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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 1.03138 -0.00003 0.00576 0.00628 0.01205 1.04343

D126 -1.03138 0.00003 -0.00576 -0.00628 -0.01205 -1.04343

D127 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D128 -2.11021 -0.00003 0.00576 0.00628 0.01205 -2.09816

D129 2.11021 0.00003 -0.00576 -0.00628 -0.01205 2.09816

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 0.004588 0.000450 NO

RMS Force 0.000882 0.000300 NO

Maximum Displacement 0.078609 0.001800 NO

RMS Displacement 0.020008 0.001200 NO

Predicted change in Energy=-1.584929D-03

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:00:13 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 -2.061216 -2.203899 0.000000

2 7 0 -0.717493 -1.888114 0.000000

3 6 0 -0.000982 -3.025068 0.000000

4 6 0 -0.899938 -4.167257 0.000000

5 6 0 -2.186415 -3.615246 0.000000

6 7 0 1.388193 -3.112916 0.000000

7 6 0 2.181431 -2.085168 0.000000

8 7 0 1.849213 -0.767897 0.000000

9 6 0 2.995664 -0.003426 0.000000

10 6 0 4.177513 -0.944821 0.000000

11 6 0 3.677709 -2.195171 0.000000

12 7 0 -3.089571 -1.277192 0.000000

13 6 0 -4.177513 0.944821 0.000000

14 6 0 -3.677709 2.195171 0.000000

15 6 0 -2.181431 2.085168 0.000000

16 7 0 -1.849213 0.767897 0.000000

17 6 0 -2.995664 0.003426 0.000000

18 7 0 -1.388193 3.112916 0.000000

19 7 0 0.717493 1.888114 0.000000

20 6 0 0.000982 3.025068 0.000000

21 6 0 0.899938 4.167257 0.000000

22 6 0 2.186415 3.615246 0.000000

23 6 0 2.061216 2.203899 0.000000

24 7 0 3.089571 1.277192 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.482943 -5.598363 0.000000

27 1 0 -3.127657 -4.154684 0.000000

28 6 0 5.593896 -0.473236 0.000000

29 1 0 4.214693 -3.135033 0.000000

30 6 0 -5.593896 0.473236 0.000000

31 1 0 -4.214693 3.135033 0.000000

32 6 0 0.482943 5.598363 0.000000

33 1 0 3.127657 4.154684 0.000000

34 1 0 -1.353652 -6.262355 0.000000

35 1 0 0.125129 -5.832950 0.889742

36 1 0 0.125129 -5.832950 -0.889742

37 1 0 5.794003 0.144347 0.890736

38 1 0 5.794003 0.144347 -0.890736

39 1 0 6.287420 -1.319952 0.000000

40 1 0 -5.794003 -0.144347 0.890736

41 1 0 -5.794003 -0.144347 -0.890736

42 1 0 -6.287420 1.319952 0.000000

43 1 0 -0.125129 5.832950 0.889742

44 1 0 -0.125129 5.832950 -0.889742

45 1 0 1.353652 6.262355 0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.380331 0.000000

3 C 2.217856 1.343894 0.000000

4 C 2.281083 2.286433 1.453520 0.000000

5 C 1.416889 2.267315 2.263720 1.399907 0.000000

6 N 3.567175 2.435990 1.391950 2.519361 3.609731

7 C 4.244308 2.905613 2.376203 3.718862 4.628090

8 N 4.165760 2.800511 2.918568 4.371896 4.938996

9 C 5.514900 4.164082 4.255609 5.702035 6.316580

10 C 6.364513 4.985066 4.667681 6.013702 6.901504

11 C 5.738932 4.405914 3.771140 4.984374 6.033620

12 N 1.384305 2.449486 3.548866 3.625875 2.506428

13 C 3.793831 4.471830 5.762242 6.072548 4.975809

14 C 4.686669 5.043422 6.385078 6.942370 5.998741

15 C 4.290752 4.234394 5.555976 6.382401 5.700416

16 N 2.979349 2.887073 4.219306 5.025622 4.396095

17 C 2.396973 2.961079 4.259096 4.667619 3.708054

18 N 5.359243 5.045805 6.292790 7.296527 6.775346

19 N 4.946291 4.039689 4.965437 6.267664 6.222512

20 C 5.620921 4.965437 6.050136 7.248531 6.991314

21 C 7.025672 6.267664 7.248531 8.526646 8.372152

22 C 7.204500 6.222512 6.991314 8.372152 8.449950

23 C 6.035158 4.946291 5.620921 7.025672 7.204500

24 N 6.216801 4.951051 5.297260 6.749683 7.195275

25 Zn 3.017579 2.019844 3.025068 4.263323 4.224975

26 C 3.743439 3.717655 2.618041 1.490621 2.614302

27 H 2.223253 3.308508 3.324474 2.227754 1.084864

28 C 7.848308 6.468037 6.149350 7.470989 8.390797

29 H 6.344608 5.087363 4.217109 5.217753 6.419096

30 C 4.432480 5.418052 6.596879 6.600561 5.322274

31 H 5.756879 6.120655 7.463391 8.019416 7.048416

32 C 8.206586 7.582110 8.636999 9.863048 9.592500

33 H 8.207069 7.162442 7.831808 9.245335 9.413350

34 H 4.119673 4.420257 3.508524 2.143663 2.775010

35 H 4.329175 4.130784 2.948176 2.148705 3.324618

36 H 4.329175 4.130784 2.948176 2.148705 3.324618

37 H 8.246948 6.879236 6.664867 8.012003 8.866511

38 H 8.246948 6.879236 6.664867 8.012003 8.866511

39 H 8.395301 7.027916 6.515475 7.730800 8.779194

40 H 4.355326 5.441056 6.530778 6.397584 5.084805

41 H 4.355326 5.441056 6.530778 6.397584 5.084805

42 H 5.502574 6.427735 7.641891 7.689891 6.416729

43 H 8.314506 7.794701 8.903456 10.069563 9.711279

44 H 8.314506 7.794701 8.903456 10.069563 9.711279

45 H 9.129008 8.409506 9.385694 10.670308 10.492810

6 7 8 9 10

6 N 0.000000

7 C 1.298265 0.000000

8 N 2.389906 1.358518 0.000000

9 C 3.500413 2.235313 1.377958 0.000000

10 C 3.532838 2.298855 2.335013 1.510957 0.000000

11 C 2.466605 1.500316 2.319593 2.295415 1.346543

12 N 4.839448 5.332569 4.964974 6.217119 7.274681

13 C 6.887838 7.043934 6.265367 7.235582 8.566050

14 C 7.337517 7.256089 6.271096 7.026218 8.459555

15 C 6.305735 6.035418 4.938225 5.582521 7.043934

16 N 5.053861 4.938225 4.004624 4.905891 6.265367

17 C 5.378642 5.582521 4.905891 5.991332 7.235582

18 N 6.816839 6.305735 5.053861 5.378642 6.887838

19 N 5.045805 4.234394 2.887073 2.961079 4.471830

20 C 6.292790 5.555976 4.219306 4.259096 5.762242

21 C 7.296527 6.382401 5.025622 4.667619 6.072548

22 C 6.775346 5.700416 4.396095 3.708054 4.975809

23 C 5.359243 4.290752 2.979349 2.396973 3.793831

24 N 4.708263 3.482842 2.391837 1.284057 2.474058

25 Zn 3.408420 3.017709 2.002312 2.995666 4.283025

26 C 3.111045 4.409244 5.363987 6.588174 6.585993

27 H 4.634456 5.698185 6.019929 7.397837 7.979269

28 C 4.965466 3.774022 3.756259 2.640365 1.492827

29 H 2.826587 2.288312 3.346465 3.360505 2.190527

30 C 7.849207 8.185422 7.545878 8.602776 9.873769

31 H 8.392210 8.255961 7.211367 7.863789 9.331363

32 C 8.758189 7.869023 6.511219 6.139529 7.514194

33 H 7.472867 6.311188 5.085885 4.160204 5.206452

34 H 4.175725 5.472267 6.359827 7.621728 7.672676

35 H 3.128187 4.366450 5.423915 6.558579 6.411494

36 H 3.128187 4.366450 5.423915 6.558579 6.411494

37 H 5.551066 4.337606 4.145717 2.940399 2.143067

38 H 5.551066 4.337606 4.145717 2.940399 2.143067

39 H 5.217005 4.176685 4.472409 3.545264 2.142995

40 H 7.822388 8.256376 7.720167 8.835809 10.043172

41 H 7.822388 8.256376 7.720167 8.835809 10.043172

42 H 8.863710 9.127775 8.400232 9.376938 10.707195

43 H 9.116485 8.295086 6.947003 6.677894 8.077286

44 H 9.116485 8.295086 6.947003 6.677894 8.077286

45 H 9.375334 8.388465 7.047696 6.477361 7.740644

11 12 13 14 15

11 C 0.000000

12 N 6.829258 0.000000

13 C 8.459555 2.474058 0.000000

14 C 8.566054 3.521820 1.346543 0.000000

15 C 7.256089 3.482842 2.298855 1.500316 0.000000

16 N 6.271096 2.391837 2.335013 2.319593 1.358518

17 C 7.026218 1.284057 1.510957 2.295415 2.235313

18 N 7.337517 4.708263 3.532838 2.466605 1.298265

19 N 5.043422 4.951051 4.985066 4.405914 2.905613

20 C 6.385078 5.297260 4.667681 3.771140 2.376203

21 C 6.942370 6.749683 6.013702 4.984374 3.718862

22 C 5.998741 7.195275 6.901504 6.033620 4.628090

23 C 4.686669 6.216801 6.364513 5.738932 4.244308

24 N 3.521820 6.686306 7.274681 6.829258 5.332569

25 Zn 4.283027 3.343153 4.283025 4.283027 3.017709

26 C 5.375197 5.046487 7.514194 8.422928 7.869023

27 H 7.081857 2.877743 5.206452 6.373634 6.311188

28 C 2.576205 8.720605 9.873769 9.647956 8.185422

29 H 1.082447 7.536833 9.331363 9.523712 8.255961

30 C 9.647956 3.055428 1.492827 2.576205 3.774022

31 H 9.523712 4.553420 2.190527 1.082447 2.288312

32 C 8.422928 7.748298 6.585993 5.375197 4.409244

33 H 6.373634 8.255859 7.979269 7.081857 5.698185

34 H 6.469666 5.278755 7.740644 8.771031 8.388465

35 H 5.161967 5.646314 8.077286 8.927706 8.295086

36 H 5.161967 5.646314 8.077286 8.927706 8.295086

37 H 3.278026 9.040580 10.043172 9.732041 8.256376

38 H 3.278026 9.040580 10.043172 9.732041 8.256376

39 H 2.752562 9.377088 10.707195 10.566924 9.127775

40 H 9.732041 3.064425 2.143067 3.278026 4.337606

41 H 9.732041 3.064425 2.143067 3.278026 4.337606

42 H 10.566924 4.119635 2.142995 2.752562 4.176685

43 H 8.927706 7.754591 6.411494 5.161967 4.366450

44 H 8.927706 7.754591 6.411494 5.161967 4.366450

45 H 8.771031 8.751400 7.672676 6.469666 5.472267

16 17 18 19 20

16 N 0.000000

17 C 1.377958 0.000000

18 N 2.389906 3.500413 0.000000

19 N 2.800511 4.164082 2.435990 0.000000

20 C 2.918568 4.255609 1.391950 1.343894 0.000000

21 C 4.371896 5.702035 2.519361 2.286433 1.453520

22 C 4.938996 6.316580 3.609731 2.267315 2.263720

23 C 4.165760 5.514900 3.567175 1.380331 2.217856

24 N 4.964974 6.217119 4.839448 2.449486 3.548866

25 Zn 2.002312 2.995666 3.408420 2.019844 3.025068

26 C 6.511219 6.139529 8.758189 7.582110 8.636999

27 H 5.085885 4.160204 7.472867 7.162442 7.831808

28 C 7.545878 8.602776 7.849207 5.418052 6.596879

29 H 7.211367 7.863789 8.392210 6.120655 7.463391

30 C 3.756259 2.640365 4.965466 6.468037 6.149350

31 H 3.346465 3.360505 2.826587 5.087363 4.217109

32 C 5.363987 6.588174 3.111045 3.717655 2.618041

33 H 6.019929 7.397837 4.634456 3.308508 3.324474

34 H 7.047696 6.477361 9.375334 8.409506 9.385694

35 H 6.947003 6.677894 9.116485 7.794701 8.903456

36 H 6.947003 6.677894 9.116485 7.794701 8.903456

37 H 7.720167 8.835809 7.822388 5.441056 6.530778

38 H 7.720167 8.835809 7.822388 5.441056 6.530778

39 H 8.400232 9.376938 8.863710 6.427735 7.641891

40 H 4.145717 2.940399 5.551066 6.879236 6.664867

41 H 4.145717 2.940399 5.551066 6.879236 6.664867

42 H 4.472409 3.545264 5.217005 7.027916 6.515475

43 H 5.423915 6.558579 3.128187 4.130784 2.948176

44 H 5.423915 6.558579 3.128187 4.130784 2.948176

45 H 6.359827 7.621728 4.175725 4.420257 3.508524

21 22 23 24 25

21 C 0.000000

22 C 1.399907 0.000000

23 C 2.281083 1.416889 0.000000

24 N 3.625875 2.506428 1.384305 0.000000

25 Zn 4.263323 4.224975 3.017579 3.343153 0.000000

26 C 9.863048 9.592500 8.206586 7.748298 5.619155

27 H 9.245335 9.413350 8.207069 8.255859 5.200349

28 C 6.600561 5.322274 4.432480 3.055428 5.613878

29 H 8.019416 7.048416 5.756879 4.553420 5.252815

30 C 7.470989 8.390797 7.848308 8.720605 5.613878

31 H 5.217753 6.419096 6.344608 7.536833 5.252815

32 C 1.490621 2.614302 3.743439 5.046487 5.619155

33 H 2.227754 1.084864 2.223253 2.877743 5.200349

34 H 10.670308 10.492810 9.129008 8.751400 6.406985

35 H 10.069563 9.711279 8.314506 7.754591 5.901745

36 H 10.069563 9.711279 8.314506 7.754591 5.901745

37 H 6.397584 5.084805 4.355326 3.064425 5.863848

38 H 6.397584 5.084805 4.355326 3.064425 5.863848

39 H 7.689891 6.416729 5.502574 4.119635 6.424478

40 H 8.012003 8.866511 8.246948 9.040580 5.863848

41 H 8.012003 8.866511 8.246948 9.040580 5.863848

42 H 7.730800 8.779194 8.395301 9.377088 6.424478

43 H 2.148705 3.324618 4.329175 5.646314 5.901745

44 H 2.148705 3.324618 4.329175 5.646314 5.901745

45 H 2.143663 2.775010 4.119673 5.278755 6.406985

26 27 28 29 30

26 C 0.000000

27 H 3.013092 0.000000

28 C 7.949522 9.466707 0.000000

29 H 5.304317 7.412813 2.997893 0.000000

30 C 7.936382 5.244041 11.227756 10.451221 0.000000

31 H 9.497272 7.370320 10.451221 10.505630 2.997893

32 C 11.238311 10.399921 7.936382 9.497272 7.949522

33 H 10.399921 10.400699 5.244041 7.370320 9.466707

34 H 1.094997 2.754881 9.043358 6.386440 7.959136

35 H 1.102915 3.766806 7.708800 4.979451 8.559606

36 H 1.102915 3.766806 7.708800 4.979451 8.559606

37 H 8.554074 9.943394 1.102208 3.747261 11.427415

38 H 8.554074 9.943394 1.102208 3.747261 11.427415

39 H 8.008908 9.832567 1.094488 2.755125 12.015872

40 H 7.664664 4.897511 11.427415 10.483874 1.102208

41 H 7.664664 4.897511 11.427415 10.483874 1.102208

42 H 9.030783 6.321055 12.015872 11.407947 1.094488

43 H 11.471469 10.467074 8.559606 10.002520 7.708800

44 H 11.471469 10.467074 8.559606 10.002520 7.708800

45 H 12.002071 11.340054 7.959136 9.823260 9.043358

31 32 33 34 35

31 H 0.000000

32 C 5.304317 0.000000

33 H 7.412813 3.013092 0.000000

34 H 9.823260 12.002071 11.340054 0.000000

35 H 10.002520 11.471469 10.467074 1.778433 0.000000

36 H 10.002520 11.471469 10.467074 1.778433 1.779484

37 H 10.483874 7.664664 4.897511 9.639928 8.237974

38 H 10.483874 7.664664 4.897511 9.639928 8.428186

39 H 11.407947 9.030783 6.321055 9.100183 7.689774

40 H 3.747261 8.554074 9.943394 7.611842 8.209526

41 H 3.747261 8.554074 9.943394 7.611842 8.400382

42 H 2.755125 8.008908 9.832567 9.046183 9.647612

43 H 4.979451 1.102915 3.766806 12.190049 11.668583

44 H 4.979451 1.102915 3.766806 12.190049 11.803491

45 H 6.386440 1.094997 2.754881 12.813970 12.190049

36 37 38 39 40

36 H 0.000000

37 H 8.428186 0.000000

38 H 8.237974 1.781472 0.000000

39 H 7.689774 1.783548 1.783548 0.000000

40 H 8.400382 11.591602 11.727697 12.171123 0.000000

41 H 8.209526 11.727697 11.591602 12.171123 1.781472

42 H 9.647612 12.171123 12.171123 12.848956 1.783548

43 H 11.803491 8.209526 8.400382 9.647612 8.237974

44 H 11.668583 8.400382 8.209526 9.647612 8.428186

45 H 12.190049 7.611842 7.611842 9.046183 9.639928

41 42 43 44 45

41 H 0.000000

42 H 1.783548 0.000000

43 H 8.428186 7.689774 0.000000

44 H 8.237974 7.689774 1.779484 0.000000

45 H 9.639928 9.100183 1.778433 1.778433 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=3 Diff= 1.05D+00

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 -2.780124 -1.173326 0.000000

2 7 0 -1.424285 -1.432196 0.000000

3 6 0 -1.232957 -2.762400 0.000000

4 6 0 -2.519170 -3.439434 0.000000

5 6 0 -3.469287 -2.411320 0.000000

6 7 0 0.000000 -3.408420 0.000000

7 6 0 1.143051 -2.792848 0.000000

8 7 0 1.376137 -1.454476 0.000000

9 6 0 2.734550 -1.223213 0.000000

10 6 0 3.430520 -2.564339 0.000000

11 6 0 2.464802 -3.502724 0.000000

12 7 0 -3.341890 0.091869 0.000000

13 6 0 -3.430520 2.564339 0.000000

14 6 0 -2.464802 3.502724 0.000000

15 6 0 -1.143051 2.792848 0.000000

16 7 0 -1.376137 1.454476 0.000000

17 6 0 -2.734550 1.223213 0.000000

18 7 0 0.000000 3.408420 0.000000

19 7 0 1.424285 1.432196 0.000000

20 6 0 1.232957 2.762400 0.000000

21 6 0 2.519170 3.439434 0.000000

22 6 0 3.469287 2.411320 0.000000

23 6 0 2.780124 1.173326 0.000000

24 7 0 3.341890 -0.091869 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -2.721193 -4.916301 0.000000

27 1 0 -4.548628 -2.520637 0.000000

28 6 0 4.916174 -2.710508 0.000000

29 1 0 2.572440 -4.579806 0.000000

30 6 0 -4.916174 2.710508 0.000000

31 1 0 -2.572440 4.579806 0.000000

32 6 0 2.721193 4.916301 0.000000

33 1 0 4.548628 2.520637 0.000000

34 1 0 -3.786846 -5.168100 0.000000

35 1 0 -2.261383 -5.378206 0.889742

36 1 0 -2.261383 -5.378206 -0.889742

37 1 0 5.350464 -2.227969 0.890736

38 1 0 5.350464 -2.227969 -0.890736

39 1 0 5.204717 -3.766276 0.000000

40 1 0 -5.350464 2.227969 0.890736

41 1 0 -5.350464 2.227969 -0.890736

42 1 0 -5.204717 3.766276 0.000000

43 1 0 2.261383 5.378206 0.889742

44 1 0 2.261383 5.378206 -0.889742

45 1 0 3.786846 5.168100 0.000000

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

Rotational constants (GHZ): 0.1831641 0.1805787 0.0911407

Leave Link 202 at Tue Sep 17 14:00:13 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 101 beta electrons

nuclear repulsion energy 2758.3940925724 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= -0.1140659595 Hartrees.

Nuclear repulsion after empirical dispersion term = 2758.2800266129 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 = 0.76D-09

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 196

GePol: Fraction of low-weight points (<1% of avg) = 5.49%

GePol: Cavity surface area = 379.526 Ang\*\*2

GePol: Cavity volume = 378.348 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0107004159 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2758.2693261970 Hartrees.

Leave Link 301 at Tue Sep 17 14:00:13 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= 15314 LenP2D= 41239.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.85D-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 14:00:14 2019, MaxMem= 2415919104 cpu: 13.4

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:00:14 2019, MaxMem= 2415919104 cpu: 1.6

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= -0.000000 -0.000000 0.000000

Rot= 0.928098 -0.000000 -0.000000 -0.372336 Ang= -43.72 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 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0340 S= 1.0113

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= -1276.13329799079

Leave Link 401 at Tue Sep 17 14:00:16 2019, MaxMem= 2415919104 cpu: 39.8

(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= 38234700.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.55D-15 for 3547.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.54D-15 for 1087 365.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.22D-15 for 3547.

Iteration 1 A^-1\*A deviation from orthogonality is 2.98D-12 for 1776 1747.

E= -1275.81904127939

DIIS: error= 5.04D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.81904127939 IErMin= 1 ErrMin= 5.04D-03

ErrMax= 5.04D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.43D-02 BMatP= 3.43D-02

IDIUse=3 WtCom= 9.50D-01 WtEn= 5.04D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.309 Goal= None Shift= 0.000

Gap= 0.393 Goal= None Shift= 0.000

GapD= 0.309 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.

RMSDP=3.25D-04 MaxDP=9.96D-03 OVMax= 1.59D-01

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.25D-04 CP: 9.99D-01

E= -1275.83302227670 Delta-E= -0.013980997313 Rises=F Damp=F

DIIS: error= 2.10D-03 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.83302227670 IErMin= 2 ErrMin= 2.10D-03

ErrMax= 2.10D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.43D-03 BMatP= 3.43D-02

IDIUse=3 WtCom= 9.79D-01 WtEn= 2.10D-02

Coeff-Com: 0.679D-01 0.932D+00

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

Coeff: 0.665D-01 0.934D+00

Gap= 0.068 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=1.10D-04 MaxDP=4.04D-03 DE=-1.40D-02 OVMax= 6.98D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 8.63D-05 CP: 9.98D-01 1.21D+00

E= -1275.83415843331 Delta-E= -0.001136156610 Rises=F Damp=F

DIIS: error= 1.50D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1275.83415843331 IErMin= 3 ErrMin= 1.50D-03

ErrMax= 1.50D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.37D-03 BMatP= 2.43D-03

IDIUse=3 WtCom= 9.85D-01 WtEn= 1.50D-02

Coeff-Com: -0.101D-01 0.410D+00 0.600D+00

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

Coeff: -0.991D-02 0.404D+00 0.606D+00

Gap= 0.069 Goal= None Shift= 0.000

Gap= 0.079 Goal= None Shift= 0.000

RMSDP=5.76D-05 MaxDP=3.13D-03 DE=-1.14D-03 OVMax= 3.54D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 5.22D-05 CP: 9.98D-01 1.28D+00 1.06D+00

E= -1275.83466107709 Delta-E= -0.000502643779 Rises=F Damp=F

DIIS: error= 8.77D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.83466107709 IErMin= 4 ErrMin= 8.77D-04

ErrMax= 8.77D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.63D-04 BMatP= 1.37D-03

IDIUse=3 WtCom= 9.91D-01 WtEn= 8.77D-03

Coeff-Com: -0.103D-01 0.900D-01 0.390D+00 0.530D+00

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

Coeff: -0.102D-01 0.892D-01 0.387D+00 0.534D+00

Gap= 0.070 Goal= None Shift= 0.000

Gap= 0.079 Goal= None Shift= 0.000

RMSDP=3.32D-05 MaxDP=1.56D-03 DE=-5.03D-04 OVMax= 2.03D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.64D-05 CP: 9.98D-01 1.33D+00 1.34D+00 1.02D+00

E= -1275.83492380934 Delta-E= -0.000262732245 Rises=F Damp=F

DIIS: error= 7.19D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.83492380934 IErMin= 5 ErrMin= 7.19D-04

ErrMax= 7.19D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.39D-05 BMatP= 5.63D-04

IDIUse=3 WtCom= 9.93D-01 WtEn= 7.19D-03

Coeff-Com: 0.913D-03-0.637D-01 0.368D-01 0.146D+00 0.880D+00

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

Coeff: 0.907D-03-0.633D-01 0.365D-01 0.145D+00 0.881D+00

Gap= 0.071 Goal= None Shift= 0.000

Gap= 0.079 Goal= None Shift= 0.000

RMSDP=3.51D-05 MaxDP=2.19D-03 DE=-2.63D-04 OVMax= 2.67D-02

Cycle 6 Pass 1 IDiag 1:

RMSU= 9.88D-06 CP: 9.98D-01 1.39D+00 1.58D+00 1.37D+00 1.25D+00

E= -1275.83506991306 Delta-E= -0.000146103717 Rises=F Damp=F

DIIS: error= 4.31D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.83506991306 IErMin= 6 ErrMin= 4.31D-04

ErrMax= 4.31D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.24D-05 BMatP= 7.39D-05

IDIUse=3 WtCom= 9.96D-01 WtEn= 4.31D-03

Coeff-Com: 0.715D-02-0.105D+00-0.227D+00-0.337D+00 0.627D+00 0.104D+01

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

Coeff: 0.712D-02-0.104D+00-0.226D+00-0.336D+00 0.624D+00 0.104D+01

Gap= 0.071 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=4.38D-05 MaxDP=2.40D-03 DE=-1.46D-04 OVMax= 3.19D-02

Cycle 7 Pass 1 IDiag 1:

RMSU= 8.22D-06 CP: 9.98D-01 1.46D+00 1.91D+00 1.74D+00 2.13D+00

CP: 1.57D+00

E= -1275.83517523330 Delta-E= -0.000105320247 Rises=F Damp=F

DIIS: error= 2.06D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.83517523330 IErMin= 7 ErrMin= 2.06D-04

ErrMax= 2.06D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.31D-05 BMatP= 6.24D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.06D-03

Coeff-Com: 0.301D-02-0.182D-01-0.933D-01-0.185D+00 0.697D-01 0.494D+00

Coeff-Com: 0.730D+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: 0.301D-02-0.181D-01-0.931D-01-0.185D+00 0.696D-01 0.493D+00

Coeff: 0.731D+00

Gap= 0.071 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=1.07D-05 MaxDP=6.42D-04 DE=-1.05D-04 OVMax= 7.24D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 3.72D-06 CP: 9.98D-01 1.47D+00 1.97D+00 1.83D+00 2.32D+00

CP: 1.99D+00 1.11D+00

E= -1275.83518738791 Delta-E= -0.000012154603 Rises=F Damp=F

DIIS: error= 1.22D-04 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.83518738791 IErMin= 8 ErrMin= 1.22D-04

ErrMax= 1.22D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.58D-06 BMatP= 1.31D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.22D-03

Coeff-Com: -0.157D-02 0.389D-01 0.448D-01 0.324D-01-0.246D+00-0.133D+00

Coeff-Com: 0.456D+00 0.808D+00

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

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

Coeff: -0.157D-02 0.389D-01 0.448D-01 0.323D-01-0.245D+00-0.133D+00

Coeff: 0.455D+00 0.808D+00

Gap= 0.071 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=6.20D-06 MaxDP=2.86D-04 DE=-1.22D-05 OVMax= 3.09D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.75D-06 CP: 9.98D-01 1.47D+00 2.00D+00 1.87D+00 2.46D+00

CP: 2.22D+00 1.42D+00 1.10D+00

E= -1275.83519244214 Delta-E= -0.000005054236 Rises=F Damp=F

DIIS: error= 4.34D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.83519244214 IErMin= 9 ErrMin= 4.34D-05

ErrMax= 4.34D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.12D-06 BMatP= 5.58D-06

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

Coeff-Com: -0.123D-02 0.196D-01 0.370D-01 0.522D-01-0.121D+00-0.144D+00

Coeff-Com: 0.558D-01 0.371D+00 0.730D+00

Coeff: -0.123D-02 0.196D-01 0.370D-01 0.522D-01-0.121D+00-0.144D+00

Coeff: 0.558D-01 0.371D+00 0.730D+00

Gap= 0.071 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=2.15D-06 MaxDP=1.14D-04 DE=-5.05D-06 OVMax= 7.06D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.13D-06 CP: 9.98D-01 1.47D+00 2.00D+00 1.89D+00 2.48D+00

CP: 2.31D+00 1.49D+00 1.39D+00 1.21D+00

E= -1275.83519336435 Delta-E= -0.000000922210 Rises=F Damp=F

DIIS: error= 2.13D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.83519336435 IErMin=10 ErrMin= 2.13D-05

ErrMax= 2.13D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.99D-07 BMatP= 1.12D-06

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

Coeff-Com: -0.258D-03 0.337D-03 0.105D-01 0.262D-01-0.482D-02-0.575D-01

Coeff-Com: -0.106D+00-0.170D-01 0.461D+00 0.688D+00

Coeff: -0.258D-03 0.337D-03 0.105D-01 0.262D-01-0.482D-02-0.575D-01

Coeff: -0.106D+00-0.170D-01 0.461D+00 0.688D+00

Gap= 0.071 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=1.52D-06 MaxDP=8.65D-05 DE=-9.22D-07 OVMax= 6.03D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 6.61D-07 CP: 9.98D-01 1.48D+00 2.00D+00 1.89D+00 2.50D+00

CP: 2.36D+00 1.56D+00 1.53D+00 1.47D+00 1.00D+00

E= -1275.83519380739 Delta-E= -0.000000443039 Rises=F Damp=F

DIIS: error= 1.19D-05 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.83519380739 IErMin=11 ErrMin= 1.19D-05

ErrMax= 1.19D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.48D-08 BMatP= 4.99D-07

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

Coeff-Com: 0.344D-03-0.669D-02-0.107D-01-0.130D-01 0.364D-01 0.335D-01

Coeff-Com: -0.267D-01-0.126D+00-0.151D+00 0.144D+00 0.112D+01

Coeff: 0.344D-03-0.669D-02-0.107D-01-0.130D-01 0.364D-01 0.335D-01

Coeff: -0.267D-01-0.126D+00-0.151D+00 0.144D+00 0.112D+01

Gap= 0.071 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=1.36D-06 MaxDP=7.78D-05 DE=-4.43D-07 OVMax= 6.60D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 3.20D-07 CP: 9.98D-01 1.48D+00 2.01D+00 1.90D+00 2.52D+00

CP: 2.39D+00 1.60D+00 1.63D+00 1.65D+00 1.39D+00

CP: 1.62D+00

E= -1275.83519397335 Delta-E= -0.000000165958 Rises=F Damp=F

DIIS: error= 6.26D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.83519397335 IErMin=12 ErrMin= 6.26D-06

ErrMax= 6.26D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.37D-08 BMatP= 7.48D-08

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

Coeff-Com: 0.233D-03-0.349D-02-0.778D-02-0.125D-01 0.207D-01 0.299D-01

Coeff-Com: 0.466D-02-0.657D-01-0.177D+00-0.812D-01 0.633D+00 0.659D+00

Coeff: 0.233D-03-0.349D-02-0.778D-02-0.125D-01 0.207D-01 0.299D-01

Coeff: 0.466D-02-0.657D-01-0.177D+00-0.812D-01 0.633D+00 0.659D+00

Gap= 0.071 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=4.63D-07 MaxDP=2.90D-05 DE=-1.66D-07 OVMax= 2.08D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.53D-07 CP: 9.98D-01 1.48D+00 2.01D+00 1.90D+00 2.53D+00

CP: 2.40D+00 1.62D+00 1.67D+00 1.72D+00 1.50D+00

CP: 1.93D+00 1.03D+00

E= -1275.83519400166 Delta-E= -0.000000028315 Rises=F Damp=F

DIIS: error= 3.33D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.83519400166 IErMin=13 ErrMin= 3.33D-06

ErrMax= 3.33D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.92D-09 BMatP= 3.37D-08

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

Coeff-Com: -0.155D-04 0.977D-03 0.454D-03-0.145D-02-0.325D-02 0.276D-02

Coeff-Com: 0.966D-02 0.133D-01-0.377D-01-0.112D+00-0.382D-01 0.373D+00

Coeff-Com: 0.793D+00

Coeff: -0.155D-04 0.977D-03 0.454D-03-0.145D-02-0.325D-02 0.276D-02

Coeff: 0.966D-02 0.133D-01-0.377D-01-0.112D+00-0.382D-01 0.373D+00

Coeff: 0.793D+00

Gap= 0.071 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=2.38D-07 MaxDP=1.68D-05 DE=-2.83D-08 OVMax= 1.31D-04

Cycle 14 Pass 1 IDiag 1:

RMSU= 9.24D-08 CP: 9.98D-01 1.48D+00 2.01D+00 1.90D+00 2.53D+00

CP: 2.41D+00 1.62D+00 1.69D+00 1.76D+00 1.57D+00

CP: 2.10D+00 1.22D+00 9.60D-01

E= -1275.83519400882 Delta-E= -0.000000007153 Rises=F Damp=F

DIIS: error= 9.61D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.83519400882 IErMin=14 ErrMin= 9.61D-07

ErrMax= 9.61D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.74D-09 BMatP= 8.92D-09

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

Coeff-Com: -0.454D-04 0.105D-02 0.143D-02 0.113D-02-0.517D-02-0.311D-02

Coeff-Com: 0.435D-02 0.185D-01 0.874D-02-0.447D-01-0.125D+00 0.799D-01

Coeff-Com: 0.416D+00 0.646D+00

Coeff: -0.454D-04 0.105D-02 0.143D-02 0.113D-02-0.517D-02-0.311D-02

Coeff: 0.435D-02 0.185D-01 0.874D-02-0.447D-01-0.125D+00 0.799D-01

Coeff: 0.416D+00 0.646D+00

Gap= 0.071 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=7.08D-08 MaxDP=4.66D-06 DE=-7.15D-09 OVMax= 3.97D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 3.59D-08 CP: 9.98D-01 1.48D+00 2.01D+00 1.90D+00 2.53D+00

CP: 2.41D+00 1.63D+00 1.70D+00 1.77D+00 1.58D+00

CP: 2.15D+00 1.27D+00 1.13D+00 1.03D+00

E= -1275.83519400967 Delta-E= -0.000000000856 Rises=F Damp=F

DIIS: error= 4.56D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.83519400967 IErMin=15 ErrMin= 4.56D-07

ErrMax= 4.56D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.34D-10 BMatP= 1.74D-09

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

Coeff-Com: -0.179D-04 0.248D-03 0.613D-03 0.101D-02-0.178D-02-0.223D-02

Coeff-Com: -0.307D-03 0.606D-02 0.132D-01 0.924D-02-0.546D-01-0.605D-01

Coeff-Com: -0.245D-02 0.299D+00 0.792D+00

Coeff: -0.179D-04 0.248D-03 0.613D-03 0.101D-02-0.178D-02-0.223D-02

Coeff: -0.307D-03 0.606D-02 0.132D-01 0.924D-02-0.546D-01-0.605D-01

Coeff: -0.245D-02 0.299D+00 0.792D+00

Gap= 0.071 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=3.52D-08 MaxDP=1.97D-06 DE=-8.56D-10 OVMax= 1.69D-05

Cycle 16 Pass 1 IDiag 1:

RMSU= 1.65D-08 CP: 9.98D-01 1.48D+00 2.01D+00 1.90D+00 2.53D+00

CP: 2.41D+00 1.63D+00 1.70D+00 1.78D+00 1.59D+00

CP: 2.16D+00 1.31D+00 1.20D+00 1.21D+00 1.09D+00

E= -1275.83519400990 Delta-E= -0.000000000227 Rises=F Damp=F

DIIS: error= 2.58D-07 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1275.83519400990 IErMin=16 ErrMin= 2.58D-07

ErrMax= 2.58D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.66D-11 BMatP= 3.34D-10

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

Coeff-Com: -0.441D-06-0.774D-04 0.445D-04 0.361D-03-0.427D-04-0.609D-03

Coeff-Com: -0.961D-03-0.800D-04 0.562D-02 0.153D-01-0.655D-02-0.495D-01

Coeff-Com: -0.835D-01 0.289D-01 0.426D+00 0.665D+00

Coeff: -0.441D-06-0.774D-04 0.445D-04 0.361D-03-0.427D-04-0.609D-03

Coeff: -0.961D-03-0.800D-04 0.562D-02 0.153D-01-0.655D-02-0.495D-01

Coeff: -0.835D-01 0.289D-01 0.426D+00 0.665D+00

Gap= 0.071 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=1.36D-08 MaxDP=9.17D-07 DE=-2.27D-10 OVMax= 5.65D-06

Cycle 17 Pass 1 IDiag 1:

RMSU= 8.04D-09 CP: 9.98D-01 1.48D+00 2.01D+00 1.90D+00 2.53D+00

CP: 2.41D+00 1.63D+00 1.70D+00 1.78D+00 1.60D+00

CP: 2.17D+00 1.31D+00 1.23D+00 1.28D+00 1.22D+00

CP: 8.87D-01

E= -1275.83519400993 Delta-E= -0.000000000033 Rises=F Damp=F

DIIS: error= 1.05D-07 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=17 EnMin= -1275.83519400993 IErMin=17 ErrMin= 1.05D-07

ErrMax= 1.05D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.60D-11 BMatP= 8.66D-11

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

Coeff-Com: 0.213D-05-0.749D-04-0.718D-04 0.435D-04 0.211D-03 0.617D-04

Coeff-Com: -0.425D-03-0.818D-03 0.768D-03 0.643D-02 0.422D-02-0.163D-01

Coeff-Com: -0.418D-01-0.272D-01 0.100D+00 0.349D+00 0.625D+00

Coeff: 0.213D-05-0.749D-04-0.718D-04 0.435D-04 0.211D-03 0.617D-04

Coeff: -0.425D-03-0.818D-03 0.768D-03 0.643D-02 0.422D-02-0.163D-01

Coeff: -0.418D-01-0.272D-01 0.100D+00 0.349D+00 0.625D+00

Gap= 0.071 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=5.61D-09 MaxDP=2.75D-07 DE=-3.32D-11 OVMax= 2.46D-06

Error on total polarization charges = 0.06503

SCF Done: E(UB3LYP) = -1275.83519401 A.U. after 17 cycles

NFock= 17 Conv=0.56D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0175 S= 1.0058

<L.S>= 0.000000000000E+00

KE= 1.320722575571D+03 PE=-8.568621479688D+03 EE= 3.213794383910D+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 2.0175, after 2.0002

Leave Link 502 at Tue Sep 17 14:01:51 2019, MaxMem= 2415919104 cpu: 1677.8

(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= 15314 LenP2D= 41239.

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 14:01:56 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 14:01:56 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 14:02:07 2019, MaxMem= 2415919104 cpu: 201.9

(Enter /home/blab/g09/l716.exe)

Dipole = 6.12843110D-14 3.87245791D-13 2.22044605D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.003439525 0.024149131 -0.000000000

2 7 -0.006809219 0.004938224 -0.000000000

3 6 0.025294232 0.007496705 0.000000000

4 6 -0.018965757 0.002198333 0.000000000

5 6 0.004327319 -0.021990770 -0.000000000

6 7 -0.029327570 -0.021606532 0.000000000

7 6 0.016406167 0.011523287 -0.000000000

8 7 0.005964205 0.004896057 0.000000000

9 6 -0.009743406 -0.028342460 -0.000000000

10 6 0.002310431 0.003790882 0.000000000

11 6 -0.007487589 0.003448681 0.000000000

12 7 -0.004217023 -0.040478922 -0.000000000

13 6 -0.002310431 -0.003790882 -0.000000000

14 6 0.007487589 -0.003448681 0.000000000

15 6 -0.016406167 -0.011523287 0.000000000

16 7 -0.005964205 -0.004896057 0.000000000

17 6 0.009743406 0.028342460 0.000000000

18 7 0.029327570 0.021606532 0.000000000

19 7 0.006809219 -0.004938224 0.000000000

20 6 -0.025294232 -0.007496705 0.000000000

21 6 0.018965757 -0.002198333 0.000000000

22 6 -0.004327319 0.021990770 -0.000000000

23 6 -0.003439525 -0.024149131 0.000000000

24 7 0.004217023 0.040478922 -0.000000000

25 30 0.000000000 0.000000000 -0.000000000

26 6 0.000387260 -0.000753089 -0.000000000

27 1 0.002497506 0.000486925 0.000000000

28 6 -0.001667848 0.000077639 -0.000000000

29 1 -0.000443890 0.000858218 0.000000000

30 6 0.001667848 -0.000077639 0.000000000

31 1 0.000443890 -0.000858218 -0.000000000

32 6 -0.000387260 0.000753089 -0.000000000

33 1 -0.002497506 -0.000486925 0.000000000

34 1 0.001875426 0.001413385 0.000000000

35 1 -0.001546948 0.000833304 -0.004934077

36 1 -0.001546948 0.000833304 0.004934077

37 1 -0.000232665 -0.001659970 -0.005070214

38 1 -0.000232665 -0.001659970 0.005070214

39 1 -0.000911524 0.002095530 0.000000000

40 1 0.000232665 0.001659970 -0.005070214

41 1 0.000232665 0.001659970 0.005070214

42 1 0.000911524 -0.002095530 0.000000000

43 1 0.001546948 -0.000833304 -0.004934077

44 1 0.001546948 -0.000833304 0.004934077

45 1 -0.001875426 -0.001413385 0.000000000

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

Cartesian Forces: Max 0.040478922 RMS 0.010031671

Leave Link 716 at Tue Sep 17 14:02:07 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 0.026171015 RMS 0.004356367

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= 5.86D-03 DEPred=-1.58D-03 R=-3.70D+00

Trust test=-3.70D+00 RLast= 3.02D-01 DXMaxT set to 1.50D-01

ITU= -1 1 1 1 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01328

Eigenvalues --- 0.01330 0.01349 0.01350 0.01602 0.01626

Eigenvalues --- 0.01627 0.01646 0.01769 0.01793 0.01802

Eigenvalues --- 0.01825 0.01879 0.01904 0.01928 0.01950

Eigenvalues --- 0.01996 0.02000 0.02041 0.02050 0.02070

Eigenvalues --- 0.02086 0.02103 0.02108 0.02115 0.02205

Eigenvalues --- 0.02313 0.02324 0.02354 0.02376 0.05382

Eigenvalues --- 0.07277 0.07277 0.07313 0.07332 0.07332

Eigenvalues --- 0.07404 0.07427 0.08522 0.14469 0.14522

Eigenvalues --- 0.15166 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16013 0.16023 0.16100

Eigenvalues --- 0.16236 0.16318 0.18494 0.19576 0.22061

Eigenvalues --- 0.22132 0.23848 0.23853 0.23890 0.24271

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25007 0.25027 0.25223

Eigenvalues --- 0.28992 0.29770 0.31211 0.33191 0.33205

Eigenvalues --- 0.33282 0.33282 0.33336 0.33454 0.33615

Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33729 0.34379 0.34437 0.34437

Eigenvalues --- 0.34439 0.35062 0.35551 0.35581 0.35599

Eigenvalues --- 0.35682 0.35682 0.35747 0.36735 0.38583

Eigenvalues --- 0.40482 0.41566 0.41934 0.43486 0.47988

Eigenvalues --- 0.48937 0.49022 0.49080 0.50842 0.51342

Eigenvalues --- 0.51377 0.52471 0.53918 0.54029 0.54324

Eigenvalues --- 0.56312 0.56386 0.56579 1.27889

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 0.10648 0.89352

Cosine: 1.000 > 0.970

Length: 1.000

GDIIS step was calculated using 2 of the last 7 vectors.

Maximum step size ( 0.150) exceeded in Quadratic search.

-- Step size scaled by 0.555

Iteration 1 RMS(Cart)= 0.00877997 RMS(Int)= 0.00006414

Iteration 2 RMS(Cart)= 0.00008305 RMS(Int)= 0.00002511

Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00002511

ITry= 1 IFail=0 DXMaxC= 4.39D-02 DCOld= 1.00D+10 DXMaxT= 1.50D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 2.07D-10 for atom 31.

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

(Linear) (Quad) (Total)

R1 2.60845 -0.00085 0.00822 -0.01399 -0.00584 2.60260

R2 2.67753 0.01218 0.02691 0.00486 0.03179 2.70932

R3 2.61596 -0.01318 -0.03548 0.00345 -0.03205 2.58391

R4 2.53959 0.00272 -0.00531 0.01327 0.00784 2.54744

R5 3.81695 -0.00003 -0.00970 0.00002 -0.00975 3.80720

R6 2.74675 0.00825 0.03196 -0.00995 0.02201 2.76877

R7 2.63040 -0.01575 -0.03052 -0.00550 -0.03605 2.59435

R8 2.64544 -0.01600 -0.02744 0.00251 -0.02488 2.62056

R9 2.81687 -0.00246 -0.00422 0.00326 -0.00096 2.81591

R10 2.05010 -0.00241 -0.00249 0.00015 -0.00234 2.04775

R11 2.45337 0.02233 0.04002 -0.00411 0.03594 2.48930

R12 2.56723 0.00168 -0.01144 0.01115 -0.00022 2.56701

R13 2.83519 -0.00627 -0.01811 -0.00722 -0.02533 2.80986

R14 2.60396 -0.00301 0.00466 -0.01109 -0.00637 2.59759

R15 3.78382 -0.00178 0.00246 0.00021 0.00276 3.78658

R16 2.85530 -0.00399 -0.02480 -0.00007 -0.02488 2.83042

R17 2.42652 0.02617 0.03341 0.00646 0.03990 2.46641

R18 2.54460 0.00036 0.00988 0.00426 0.01413 2.55873

R19 2.82103 -0.00324 -0.00332 0.00087 -0.00245 2.81858

R20 2.04553 -0.00097 -0.00107 0.00068 -0.00039 2.04514

R21 2.42652 0.02617 0.03341 0.00646 0.03990 2.46641

R22 2.54460 0.00036 0.00988 0.00426 0.01413 2.55873

R23 2.85530 -0.00399 -0.02480 -0.00007 -0.02488 2.83042

R24 2.82103 -0.00324 -0.00332 0.00087 -0.00245 2.81858

R25 2.83519 -0.00627 -0.01811 -0.00722 -0.02533 2.80986

R26 2.04553 -0.00097 -0.00107 0.00068 -0.00039 2.04514

R27 2.56723 0.00168 -0.01144 0.01115 -0.00022 2.56701

R28 2.45337 0.02233 0.04002 -0.00411 0.03594 2.48930

R29 2.60396 -0.00301 0.00466 -0.01109 -0.00637 2.59759

R30 3.78382 -0.00178 0.00246 0.00021 0.00276 3.78658

R31 2.63040 -0.01575 -0.03052 -0.00550 -0.03605 2.59435

R32 2.53959 0.00272 -0.00531 0.01327 0.00784 2.54744

R33 2.60845 -0.00085 0.00822 -0.01399 -0.00584 2.60260

R34 3.81695 -0.00003 -0.00970 0.00002 -0.00975 3.80720

R35 2.74675 0.00825 0.03196 -0.00995 0.02201 2.76877

R36 2.64544 -0.01600 -0.02744 0.00251 -0.02488 2.62056

R37 2.81687 -0.00246 -0.00422 0.00326 -0.00096 2.81591

R38 2.67753 0.01218 0.02691 0.00486 0.03179 2.70932

R39 2.05010 -0.00241 -0.00249 0.00015 -0.00234 2.04775

R40 2.61596 -0.01318 -0.03548 0.00345 -0.03205 2.58391

R41 2.06925 -0.00235 -0.00276 0.00065 -0.00211 2.06713

R42 2.08421 -0.00501 -0.00548 0.00124 -0.00424 2.07997

R43 2.08421 -0.00501 -0.00548 0.00124 -0.00424 2.07997

R44 2.08287 -0.00507 -0.00546 0.00148 -0.00398 2.07889

R45 2.08287 -0.00507 -0.00546 0.00148 -0.00398 2.07889

R46 2.06828 -0.00220 -0.00251 0.00073 -0.00178 2.06650

R47 2.08287 -0.00507 -0.00546 0.00148 -0.00398 2.07889

R48 2.08287 -0.00507 -0.00546 0.00148 -0.00398 2.07889

R49 2.06828 -0.00220 -0.00251 0.00073 -0.00178 2.06650

R50 2.08421 -0.00501 -0.00548 0.00124 -0.00424 2.07997

R51 2.08421 -0.00501 -0.00548 0.00124 -0.00424 2.07997

R52 2.06925 -0.00235 -0.00276 0.00065 -0.00211 2.06713

A1 1.89009 0.00267 -0.00334 0.00302 -0.00033 1.88976

A2 2.17732 0.00414 0.01108 0.00233 0.01336 2.19068

A3 2.21577 -0.00681 -0.00774 -0.00535 -0.01303 2.20274

A4 1.90231 -0.00363 0.00448 -0.00215 0.00232 1.90463

A5 2.16477 0.00475 0.00625 0.00277 0.00905 2.17382

A6 2.21611 -0.00112 -0.01074 -0.00062 -0.01137 2.20474

A7 1.91247 -0.00134 -0.00847 0.00109 -0.00740 1.90507

A8 2.19628 0.00497 0.02031 -0.00724 0.01300 2.20928

A9 2.17444 -0.00363 -0.01184 0.00615 -0.00560 2.16884

A10 1.83226 0.00487 0.00863 -0.00002 0.00862 1.84089

A11 2.19127 -0.00256 -0.01405 0.00580 -0.00826 2.18301

A12 2.25965 -0.00230 0.00542 -0.00578 -0.00037 2.25929

A13 1.88765 -0.00257 -0.00130 -0.00195 -0.00322 1.88443

A14 2.17969 0.00213 -0.00300 0.00235 -0.00066 2.17902

A15 2.21585 0.00044 0.00430 -0.00040 0.00388 2.21973

A16 2.16496 -0.00371 -0.00927 0.01174 0.00244 2.16740

A17 2.23722 0.00026 -0.00297 -0.00440 -0.00731 2.22991

A18 2.15473 0.00295 0.00310 0.00487 0.00791 2.16264

A19 1.89123 -0.00321 -0.00013 -0.00048 -0.00060 1.89063

A20 1.91185 0.00237 -0.00039 -0.00094 -0.00136 1.91049

A21 2.21144 -0.00293 -0.00447 -0.00294 -0.00737 2.20407

A22 2.15990 0.00056 0.00486 0.00387 0.00873 2.16862

A23 1.88086 -0.00105 0.00172 0.00271 0.00444 1.88530

A24 2.23210 0.00343 -0.00261 -0.00076 -0.00333 2.22877

A25 2.17023 -0.00238 0.00089 -0.00195 -0.00111 2.16912

A26 1.86315 -0.00062 -0.00324 -0.00094 -0.00417 1.85898

A27 2.14756 0.00015 0.00722 0.00322 0.01044 2.15800

A28 2.27248 0.00047 -0.00398 -0.00229 -0.00627 2.26621

A29 1.87769 0.00251 0.00203 -0.00036 0.00169 1.87938

A30 2.16326 -0.00121 0.00261 0.00207 0.00468 2.16794

A31 2.24224 -0.00130 -0.00465 -0.00171 -0.00637 2.23587

A32 2.23105 -0.01035 -0.01244 -0.00475 -0.01719 2.21386

A33 1.86315 -0.00062 -0.00324 -0.00094 -0.00417 1.85898

A34 2.27248 0.00047 -0.00398 -0.00229 -0.00627 2.26621

A35 2.14756 0.00015 0.00722 0.00322 0.01044 2.15800

A36 1.87769 0.00251 0.00203 -0.00036 0.00169 1.87938

A37 2.24224 -0.00130 -0.00465 -0.00171 -0.00637 2.23587

A38 2.16326 -0.00121 0.00261 0.00207 0.00468 2.16794

A39 1.89123 -0.00321 -0.00013 -0.00048 -0.00060 1.89063

A40 2.15473 0.00295 0.00310 0.00487 0.00791 2.16264

A41 2.23722 0.00026 -0.00297 -0.00440 -0.00731 2.22991

A42 1.91185 0.00237 -0.00039 -0.00094 -0.00136 1.91049

A43 2.21144 -0.00293 -0.00447 -0.00294 -0.00737 2.20407

A44 2.15990 0.00056 0.00486 0.00387 0.00873 2.16862

A45 2.17023 -0.00238 0.00089 -0.00195 -0.00111 2.16912

A46 2.23210 0.00343 -0.00261 -0.00076 -0.00333 2.22877

A47 1.88086 -0.00105 0.00172 0.00271 0.00444 1.88530

A48 2.16496 -0.00371 -0.00927 0.01174 0.00244 2.16740

A49 1.90231 -0.00363 0.00448 -0.00215 0.00232 1.90463

A50 2.21611 -0.00112 -0.01074 -0.00062 -0.01137 2.20474

A51 2.16477 0.00475 0.00625 0.00277 0.00905 2.17382

A52 2.19628 0.00497 0.02031 -0.00724 0.01300 2.20928

A53 2.17444 -0.00363 -0.01184 0.00615 -0.00560 2.16884

A54 1.91247 -0.00134 -0.00847 0.00109 -0.00740 1.90507

A55 1.83226 0.00487 0.00863 -0.00002 0.00862 1.84089

A56 2.19127 -0.00256 -0.01405 0.00580 -0.00826 2.18301

A57 2.25965 -0.00230 0.00542 -0.00578 -0.00037 2.25929

A58 1.88765 -0.00257 -0.00130 -0.00195 -0.00322 1.88443

A59 2.21585 0.00044 0.00430 -0.00040 0.00388 2.21973

A60 2.17969 0.00213 -0.00300 0.00235 -0.00066 2.17902

A61 1.89009 0.00267 -0.00334 0.00302 -0.00033 1.88976

A62 2.17732 0.00414 0.01108 0.00233 0.01336 2.19068

A63 2.21577 -0.00681 -0.00774 -0.00535 -0.01303 2.20274

A64 2.23105 -0.01035 -0.01244 -0.00475 -0.01719 2.21386

A65 1.54036 0.00252 0.00714 0.00345 0.01061 1.55097

A66 1.60123 -0.00252 -0.00714 -0.00345 -0.01061 1.59063

A67 1.60123 -0.00252 -0.00714 -0.00345 -0.01061 1.59063

A68 1.54036 0.00252 0.00714 0.00345 0.01061 1.55097

A69 1.93877 0.00021 0.00359 -0.00331 0.00030 1.93907

A70 1.93739 0.00050 -0.00033 0.00024 -0.00007 1.93732

A71 1.93739 0.00050 -0.00033 0.00024 -0.00007 1.93732

A72 1.88539 0.00016 0.00297 -0.00050 0.00249 1.88787

A73 1.88539 0.00016 0.00297 -0.00050 0.00249 1.88787

A74 1.87715 -0.00160 -0.00920 0.00400 -0.00518 1.87197

A75 1.92758 0.00100 0.00400 -0.00039 0.00362 1.93120

A76 1.92758 0.00100 0.00400 -0.00039 0.00362 1.93120

A77 1.93565 0.00082 0.00333 -0.00210 0.00125 1.93690

A78 1.88197 -0.00202 -0.00946 0.00304 -0.00642 1.87555

A79 1.89487 -0.00046 -0.00124 -0.00000 -0.00123 1.89364

A80 1.89487 -0.00046 -0.00124 -0.00000 -0.00123 1.89364

A81 1.92758 0.00100 0.00400 -0.00039 0.00362 1.93120

A82 1.92758 0.00100 0.00400 -0.00039 0.00362 1.93120

A83 1.93565 0.00082 0.00333 -0.00210 0.00125 1.93690

A84 1.88197 -0.00202 -0.00946 0.00304 -0.00642 1.87555

A85 1.89487 -0.00046 -0.00124 -0.00000 -0.00123 1.89364

A86 1.89487 -0.00046 -0.00124 -0.00000 -0.00123 1.89364

A87 1.93739 0.00050 -0.00033 0.00024 -0.00007 1.93732

A88 1.93739 0.00050 -0.00033 0.00024 -0.00007 1.93732

A89 1.93877 0.00021 0.00359 -0.00331 0.00030 1.93907

A90 1.87715 -0.00160 -0.00920 0.00400 -0.00518 1.87197

A91 1.88539 0.00016 0.00297 -0.00050 0.00249 1.88787

A92 1.88539 0.00016 0.00297 -0.00050 0.00249 1.88787

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

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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 1.04343 -0.00067 -0.00598 0.00268 -0.00330 1.04013

D31 -1.04343 0.00067 0.00598 -0.00268 0.00330 -1.04013

D32 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D33 -2.09816 -0.00067 -0.00598 0.00268 -0.00330 -2.10146

D34 2.09816 0.00067 0.00598 -0.00268 0.00330 2.10146

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

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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

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 1.04009 -0.00062 -0.00333 0.00164 -0.00169 1.03840

D64 -1.04009 0.00062 0.00333 -0.00164 0.00169 -1.03840

D65 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

D66 -2.10150 -0.00062 -0.00333 0.00164 -0.00169 -2.10319

D67 2.10150 0.00062 0.00333 -0.00164 0.00169 2.10319

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 -2.10150 -0.00062 -0.00333 0.00164 -0.00169 -2.10319

D80 2.10150 0.00062 0.00333 -0.00164 0.00169 2.10319

D81 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D82 1.04009 -0.00062 -0.00333 0.00164 -0.00169 1.03840

D83 -1.04009 0.00062 0.00333 -0.00164 0.00169 -1.03840

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

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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

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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 1.04343 -0.00067 -0.00598 0.00268 -0.00330 1.04013

D126 -1.04343 0.00067 0.00598 -0.00268 0.00330 -1.04013

D127 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D128 -2.09816 -0.00067 -0.00598 0.00268 -0.00330 -2.10146

D129 2.09816 0.00067 0.00598 -0.00268 0.00330 2.10146

D130 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 0.026171 0.000450 NO

RMS Force 0.004356 0.000300 NO

Maximum Displacement 0.043901 0.001800 NO

RMS Displacement 0.008781 0.001200 NO

Predicted change in Energy=-7.052769D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:02:07 2019, MaxMem= 2415919104 cpu: 1.5

(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 -2.066082 -2.198703 0.000000

2 7 0 -0.726424 -1.879166 0.000000

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6 7 0 1.368193 -3.112259 0.000000

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9 6 0 3.000861 -0.001202 0.000000

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11 6 0 3.665919 -2.189183 0.000000

12 7 0 -3.096970 -1.300424 0.000000

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25 30 0 0.000000 0.000000 0.000000

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27 1 0 -3.126096 -4.168891 0.000000

28 6 0 5.592694 -0.476452 0.000000

29 1 0 4.205434 -3.127356 0.000000

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36 1 0 0.127859 -5.822429 -0.886243

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Distance matrix (angstroms):

1 2 3 4 5

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2 N 1.377239 0.000000

3 C 2.220519 1.348045 0.000000

4 C 2.281523 2.293454 1.465167 0.000000

5 C 1.433712 2.278314 2.270244 1.386740 0.000000

6 N 3.553707 2.430625 1.372870 2.509288 3.592842

7 C 4.251030 2.916384 2.377420 3.731481 4.637422

8 N 4.176232 2.813176 2.921180 4.386157 4.955911

9 C 5.522945 4.173655 4.254300 5.712287 6.329918

10 C 6.366013 4.989795 4.664597 6.022817 6.907358

11 C 5.732009 4.403270 3.759140 4.983872 6.027530

12 N 1.367346 2.440171 3.539074 3.604558 2.498243

13 C 3.775033 4.448693 5.744533 6.053958 4.974352

14 C 4.670441 5.019172 6.365448 6.926594 6.001383

15 C 4.277690 4.216222 5.540658 6.371317 5.704645

16 N 2.965681 2.869522 4.205237 5.014533 4.399307

17 C 2.390270 2.951075 4.254217 4.661955 3.718497

18 N 5.356618 5.032513 6.278419 7.292010 6.789143

19 N 4.942378 4.029370 4.948514 6.261924 6.229924

20 C 5.609134 4.948514 6.031104 7.238377 6.994130

21 C 7.025265 6.261924 7.238377 8.526865 8.385429

22 C 7.213543 6.229924 6.994130 8.385429 8.471689

23 C 6.034232 4.942378 5.609134 7.025265 7.213543

24 N 6.237066 4.972739 5.312882 6.776838 7.225524

25 Zn 3.017116 2.014685 3.015552 4.263433 4.235844

26 C 3.745361 3.721966 2.622312 1.490113 2.601798

27 H 2.237246 3.316815 3.330878 2.216658 1.083623

28 C 7.850032 6.472933 6.143242 7.475654 8.394030

29 H 6.339898 5.087357 4.208186 5.219126 6.412496

30 C 4.426449 5.406433 6.592280 6.593845 5.332494

31 H 5.739663 6.096620 7.443812 8.002906 7.049590

32 C 8.198338 7.569635 8.622359 9.857372 9.599474

33 H 8.216140 7.170836 7.835599 9.259827 9.434764

34 H 4.126554 4.427167 3.515288 2.142577 2.765472

35 H 4.327840 4.130926 2.946296 2.146502 3.311389

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37 H 8.255830 6.890612 6.664726 8.022562 8.877337

38 H 8.255830 6.890612 6.664726 8.022562 8.877337

39 H 8.389682 7.026380 6.502307 7.727378 8.772461

40 H 4.356717 5.437934 6.534698 6.397340 5.100136

41 H 4.356717 5.437934 6.534698 6.397340 5.100136

42 H 5.493926 6.411857 7.633552 7.681495 6.425939

43 H 8.299439 7.775492 8.883206 10.057393 9.712074

44 H 8.299439 7.775492 8.883206 10.057393 9.712074

45 H 9.124150 8.401826 9.375630 10.669380 10.502833

6 7 8 9 10

6 N 0.000000

7 C 1.317281 0.000000

8 N 2.402541 1.358401 0.000000

9 C 3.513442 2.231383 1.374588 0.000000

10 C 3.551476 2.295035 2.325224 1.497794 0.000000

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12 N 4.818758 5.337044 4.980734 6.234703 7.279191

13 C 6.861067 7.033331 6.260555 7.234498 8.552311

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16 N 5.037282 4.934456 4.007544 4.914371 6.260555

17 C 5.364911 5.585264 4.914371 6.001722 7.234498

18 N 6.799443 6.288473 5.037282 5.364911 6.861067

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23 C 5.356618 4.277690 2.965681 2.390270 3.775033

24 N 4.739244 3.499218 2.405649 1.305169 2.479727

25 Zn 3.399722 3.013628 2.003772 3.000861 4.276156

26 C 3.095635 4.412604 5.369325 6.588590 6.587235

27 H 4.616828 5.706417 6.035632 7.410076 7.983921

28 C 4.979346 3.766632 3.749094 2.635045 1.491530

29 H 2.837281 2.278554 3.336922 3.350200 2.193909

30 C 7.831526 8.184550 7.548839 8.606819 9.866956

31 H 8.366488 8.240399 7.199113 7.856116 9.310738

32 C 8.750300 7.856674 6.498849 6.134762 7.497589

33 H 7.490351 6.317037 5.089754 4.171973 5.208864

34 H 4.159831 5.476120 6.367203 7.623657 7.673504

35 H 3.109482 4.362945 5.422195 6.551813 6.406887

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37 H 5.569521 4.335527 4.144633 2.941380 2.142931

38 H 5.569521 4.335527 4.144633 2.941380 2.142931

39 H 5.224153 4.163054 4.460475 3.535982 2.142030

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42 H 8.842423 9.121233 8.396331 9.373962 10.693303

43 H 9.102321 8.278498 6.930723 6.670007 8.057774

44 H 9.102321 8.278498 6.930723 6.670007 8.057774

45 H 9.374679 8.381444 7.039994 6.477867 7.730520

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19 N 5.019172 4.972739 4.989795 4.403270 2.916384

20 C 6.365448 5.312882 4.664597 3.759140 2.377420

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25 Zn 4.269834 3.358918 4.276156 4.269834 3.013628

26 C 5.366853 5.025845 7.497589 8.407993 7.856674

27 H 7.074652 2.868615 5.208864 6.380949 6.317037

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34 H 6.460357 5.260998 7.730520 8.763523 8.381444

35 H 5.148182 5.624365 8.057774 8.908653 8.278498

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37 H 3.282220 9.058079 10.045526 9.727473 8.264434

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43 H 8.908653 7.767631 6.406887 5.148182 4.362945

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16 17 18 19 20

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22 C 4.955911 6.329918 3.592842 2.278314 2.270244

23 C 4.176232 5.522945 3.553707 1.377239 2.220519

24 N 4.980734 6.234703 4.818758 2.440171 3.539074

25 Zn 2.003772 3.000861 3.399722 2.014685 3.015552

26 C 6.498849 6.134762 8.750300 7.569635 8.622359

27 H 5.089754 4.171973 7.490351 7.170836 7.835599

28 C 7.548839 8.606819 7.831526 5.406433 6.592280

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31 H 3.336922 3.350200 2.837281 5.087357 4.208186

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34 H 7.039994 6.477867 9.374679 8.401826 9.375630

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36 H 6.930723 6.670007 9.102321 7.775492 8.883206

37 H 7.732138 8.848297 7.812195 5.437934 6.534698

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37 H 6.397340 5.100136 4.356717 3.074020 5.870849

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39 H 7.681495 6.425939 5.493926 4.126932 6.417321

40 H 8.022562 8.877337 8.255830 9.058079 5.870849

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42 H 7.727378 8.772461 8.389682 9.375345 6.417321

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26 27 28 29 30

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34 H 1.093879 2.746338 9.036501 6.377733 7.963963

35 H 1.100672 3.756040 7.696059 4.967440 8.554885

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37 H 8.553149 9.952832 1.100101 3.742944 11.433897

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39 H 7.994261 9.824048 1.093547 2.744687 12.007441

40 H 7.668890 4.917228 11.433897 10.481230 1.100101

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42 H 9.027197 6.336904 12.007441 11.391346 1.093547

43 H 11.455476 10.469065 8.554885 9.983062 7.696059

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39 H 11.391346 9.027197 6.336904 9.083746 7.668796

40 H 3.742944 8.553149 9.952832 7.622555 8.212936

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42 H 2.744687 7.994261 9.824048 9.051086 9.641498

43 H 4.967440 1.100672 3.756040 12.178614 11.647666

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45 H 6.377733 1.093879 2.746338 12.811915 12.178614

36 37 38 39 40

36 H 0.000000

37 H 8.419403 0.000000

38 H 8.230561 1.773897 0.000000

39 H 7.668796 1.780285 1.780285 0.000000

40 H 8.402174 11.606928 11.741698 12.170799 0.000000

41 H 8.212936 11.741698 11.606928 12.170799 1.773897

42 H 9.641498 12.170799 12.170799 12.834641 1.780285

43 H 11.781758 8.212936 8.402174 9.641498 8.230561

44 H 11.647666 8.402174 8.212936 9.641498 8.419403

45 H 12.178614 7.622555 7.622555 9.051086 9.638619

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41 H 0.000000

42 H 1.780285 0.000000

43 H 8.419403 7.668796 0.000000

44 H 8.230561 7.668796 1.772485 0.000000

45 H 9.638619 9.083746 1.777314 1.777314 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=3 Diff= 7.49D-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

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40 1 0 -5.367492 2.206859 0.886949

41 1 0 -5.367492 2.206859 -0.886949

42 1 0 -5.212882 3.742709 0.000000

43 1 0 2.226147 5.381571 0.886243

44 1 0 2.226147 5.381571 -0.886243

45 1 0 3.754800 5.190160 0.000000

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

Rotational constants (GHZ): 0.1827374 0.1812820 0.0912116

Leave Link 202 at Tue Sep 17 14:02:07 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 101 beta electrons

nuclear repulsion energy 2759.1868171124 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= -0.1140953874 Hartrees.

Nuclear repulsion after empirical dispersion term = 2759.0727217250 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 = 3584

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.75D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 230

GePol: Fraction of low-weight points (<1% of avg) = 6.42%

GePol: Cavity surface area = 379.134 Ang\*\*2

GePol: Cavity volume = 378.313 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0107071461 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2759.0620145789 Hartrees.

Leave Link 301 at Tue Sep 17 14:02:07 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= 15317 LenP2D= 41236.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.85D-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 14:02:08 2019, MaxMem= 2415919104 cpu: 13.7

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:02:08 2019, MaxMem= 2415919104 cpu: 1.3

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999997 -0.000000 0.000000 -0.002644 Ang= -0.30 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 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0175 S= 1.0058

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= -1276.13999836731

Leave Link 401 at Tue Sep 17 14:02:10 2019, MaxMem= 2415919104 cpu: 40.2

(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= 38535168.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.00D-15 for 3574.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.77D-15 for 3583 1338.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.00D-15 for 3574.

Iteration 1 A^-1\*A deviation from orthogonality is 3.78D-13 for 2009 1980.

E= -1275.83860071849

DIIS: error= 2.52D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.83860071849 IErMin= 1 ErrMin= 2.52D-03

ErrMax= 2.52D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.64D-03 BMatP= 8.64D-03

IDIUse=3 WtCom= 9.75D-01 WtEn= 2.52D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.307 Goal= None Shift= 0.000

Gap= 0.392 Goal= None Shift= 0.000

GapD= 0.307 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.

RMSDP=1.31D-04 MaxDP=3.36D-03 OVMax= 3.18D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.31D-04 CP: 1.00D+00

E= -1275.84141948756 Delta-E= -0.002818769076 Rises=F Damp=F

DIIS: error= 7.39D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84141948756 IErMin= 2 ErrMin= 7.39D-04

ErrMax= 7.39D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.44D-04 BMatP= 8.64D-03

IDIUse=3 WtCom= 9.93D-01 WtEn= 7.39D-03

Coeff-Com: 0.828D-01 0.917D+00

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

Coeff: 0.821D-01 0.918D+00

Gap= 0.057 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=3.93D-05 MaxDP=2.10D-03 DE=-2.82D-03 OVMax= 1.04D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.74D-05 CP: 1.00D+00 1.09D+00

E= -1275.84141840608 Delta-E= 0.000001081479 Rises=F Damp=F

DIIS: error= 6.91D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1275.84141948756 IErMin= 3 ErrMin= 6.91D-04

ErrMax= 6.91D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.26D-04 BMatP= 6.44D-04

IDIUse=3 WtCom= 2.76D-01 WtEn= 7.24D-01

Coeff-Com: -0.663D-02 0.519D+00 0.488D+00

Coeff-En: 0.000D+00 0.502D+00 0.498D+00

Coeff: -0.183D-02 0.507D+00 0.495D+00

Gap= 0.057 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=2.80D-05 MaxDP=1.46D-03 DE= 1.08D-06 OVMax= 7.40D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.67D-05 CP: 1.00D+00 1.10D+00 4.01D-01

E= -1275.84157102432 Delta-E= -0.000152618240 Rises=F Damp=F

DIIS: error= 3.27D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84157102432 IErMin= 4 ErrMin= 3.27D-04

ErrMax= 3.27D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.04D-04 BMatP= 6.44D-04

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

Coeff-Com: -0.101D-01 0.149D+00 0.301D+00 0.560D+00

Coeff-En: 0.000D+00 0.000D+00 0.985D-01 0.901D+00

Coeff: -0.101D-01 0.149D+00 0.300D+00 0.561D+00

Gap= 0.057 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=9.42D-06 MaxDP=4.68D-04 DE=-1.53D-04 OVMax= 1.83D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 6.70D-06 CP: 1.00D+00 1.11D+00 5.60D-01 8.44D-01

E= -1275.84159703994 Delta-E= -0.000026015618 Rises=F Damp=F

DIIS: error= 1.25D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84159703994 IErMin= 5 ErrMin= 1.25D-04

ErrMax= 1.25D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.80D-06 BMatP= 1.04D-04

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.25D-03

Coeff-Com: -0.412D-02 0.359D-01 0.132D+00 0.297D+00 0.539D+00

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

Coeff: -0.412D-02 0.358D-01 0.132D+00 0.296D+00 0.540D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=4.17D-06 MaxDP=2.32D-04 DE=-2.60D-05 OVMax= 2.26D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.68D-06 CP: 1.00D+00 1.12D+00 5.73D-01 1.03D+00 9.75D-01

E= -1275.84160111735 Delta-E= -0.000004077407 Rises=F Damp=F

DIIS: error= 5.91D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84160111735 IErMin= 6 ErrMin= 5.91D-05

ErrMax= 5.91D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.41D-06 BMatP= 8.80D-06

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

Coeff-Com: 0.204D-02-0.455D-01-0.489D-01-0.107D+00 0.254D+00 0.946D+00

Coeff: 0.204D-02-0.455D-01-0.489D-01-0.107D+00 0.254D+00 0.946D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=4.57D-06 MaxDP=2.19D-04 DE=-4.08D-06 OVMax= 2.61D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.63D-06 CP: 1.00D+00 1.12D+00 6.06D-01 1.18D+00 1.39D+00

CP: 1.38D+00

E= -1275.84160390258 Delta-E= -0.000002785236 Rises=F Damp=F

DIIS: error= 3.41D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84160390258 IErMin= 7 ErrMin= 3.41D-05

ErrMax= 3.41D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.65D-07 BMatP= 2.41D-06

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

Coeff-Com: 0.233D-02-0.350D-01-0.620D-01-0.156D+00 0.627D-03 0.462D+00

Coeff-Com: 0.787D+00

Coeff: 0.233D-02-0.350D-01-0.620D-01-0.156D+00 0.627D-03 0.462D+00

Coeff: 0.787D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=3.02D-06 MaxDP=1.60D-04 DE=-2.79D-06 OVMax= 1.97D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 8.83D-07 CP: 1.00D+00 1.13D+00 6.21D-01 1.29D+00 1.63D+00

CP: 1.85D+00 1.35D+00

E= -1275.84160476076 Delta-E= -0.000000858174 Rises=F Damp=F

DIIS: error= 1.91D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84160476076 IErMin= 8 ErrMin= 1.91D-05

ErrMax= 1.91D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.77D-07 BMatP= 6.65D-07

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

Coeff-Com: 0.557D-03-0.258D-02-0.146D-01-0.529D-01-0.699D-01-0.931D-01

Coeff-Com: 0.475D+00 0.757D+00

Coeff: 0.557D-03-0.258D-02-0.146D-01-0.529D-01-0.699D-01-0.931D-01

Coeff: 0.475D+00 0.757D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=1.72D-06 MaxDP=9.50D-05 DE=-8.58D-07 OVMax= 1.14D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 4.53D-07 CP: 1.00D+00 1.13D+00 6.28D-01 1.34D+00 1.77D+00

CP: 2.09D+00 1.78D+00 1.14D+00

E= -1275.84160501515 Delta-E= -0.000000254393 Rises=F Damp=F

DIIS: error= 9.39D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84160501515 IErMin= 9 ErrMin= 9.39D-06

ErrMax= 9.39D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.48D-08 BMatP= 2.77D-07

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

Coeff-Com: -0.320D-03 0.828D-02 0.992D-02 0.114D-01-0.290D-01-0.180D+00

Coeff-Com: 0.713D-01 0.391D+00 0.718D+00

Coeff: -0.320D-03 0.828D-02 0.992D-02 0.114D-01-0.290D-01-0.180D+00

Coeff: 0.713D-01 0.391D+00 0.718D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=7.76D-07 MaxDP=4.19D-05 DE=-2.54D-07 OVMax= 5.52D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 2.81D-07 CP: 1.00D+00 1.13D+00 6.30D-01 1.37D+00 1.82D+00

CP: 2.22D+00 1.97D+00 1.44D+00 1.22D+00

E= -1275.84160507675 Delta-E= -0.000000061598 Rises=F Damp=F

DIIS: error= 6.30D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84160507675 IErMin=10 ErrMin= 6.30D-06

ErrMax= 6.30D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.00D-08 BMatP= 6.48D-08

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

Coeff-Com: -0.303D-03 0.417D-02 0.961D-02 0.208D-01 0.179D-01-0.483D-01

Coeff-Com: -0.111D+00-0.106D+00 0.341D+00 0.872D+00

Coeff: -0.303D-03 0.417D-02 0.961D-02 0.208D-01 0.179D-01-0.483D-01

Coeff: -0.111D+00-0.106D+00 0.341D+00 0.872D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=5.27D-07 MaxDP=2.78D-05 DE=-6.16D-08 OVMax= 3.85D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.44D-07 CP: 1.00D+00 1.13D+00 6.31D-01 1.38D+00 1.84D+00

CP: 2.29D+00 2.11D+00 1.65D+00 1.73D+00 1.40D+00

E= -1275.84160510439 Delta-E= -0.000000027643 Rises=F Damp=F

DIIS: error= 4.12D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84160510439 IErMin=11 ErrMin= 4.12D-06

ErrMax= 4.12D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.33D-09 BMatP= 2.00D-08

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

Coeff-Com: -0.231D-04-0.904D-03 0.964D-03 0.361D-02 0.170D-01 0.223D-01

Coeff-Com: -0.477D-01-0.155D+00-0.566D-01 0.324D+00 0.892D+00

Coeff: -0.231D-04-0.904D-03 0.964D-03 0.361D-02 0.170D-01 0.223D-01

Coeff: -0.477D-01-0.155D+00-0.566D-01 0.324D+00 0.892D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=3.63D-07 MaxDP=2.10D-05 DE=-2.76D-08 OVMax= 2.68D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 8.32D-08 CP: 1.00D+00 1.13D+00 6.31D-01 1.38D+00 1.86D+00

CP: 2.34D+00 2.19D+00 1.79D+00 2.06D+00 1.88D+00

CP: 1.53D+00

E= -1275.84160511621 Delta-E= -0.000000011815 Rises=F Damp=F

DIIS: error= 2.81D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84160511621 IErMin=12 ErrMin= 2.81D-06

ErrMax= 2.81D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.88D-09 BMatP= 6.33D-09

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

Coeff-Com: 0.112D-03-0.238D-02-0.324D-02-0.677D-02 0.580D-02 0.310D-01

Coeff-Com: 0.220D-01-0.631D-01-0.172D+00-0.139D+00 0.492D+00 0.835D+00

Coeff: 0.112D-03-0.238D-02-0.324D-02-0.677D-02 0.580D-02 0.310D-01

Coeff: 0.220D-01-0.631D-01-0.172D+00-0.139D+00 0.492D+00 0.835D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=2.90D-07 MaxDP=1.45D-05 DE=-1.18D-08 OVMax= 2.14D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 5.32D-08 CP: 1.00D+00 1.13D+00 6.32D-01 1.39D+00 1.87D+00

CP: 2.37D+00 2.24D+00 1.89D+00 2.32D+00 2.26D+00

CP: 2.22D+00 1.38D+00

E= -1275.84160512232 Delta-E= -0.000000006113 Rises=F Damp=F

DIIS: error= 1.53D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84160512232 IErMin=13 ErrMin= 1.53D-06

ErrMax= 1.53D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.29D-09 BMatP= 2.88D-09

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

Coeff-Com: 0.587D-04-0.662D-03-0.162D-02-0.468D-02-0.313D-02 0.194D-02

Coeff-Com: 0.335D-01 0.304D-01-0.482D-01-0.185D+00-0.214D+00 0.466D+00

Coeff-Com: 0.925D+00

Coeff: 0.587D-04-0.662D-03-0.162D-02-0.468D-02-0.313D-02 0.194D-02

Coeff: 0.335D-01 0.304D-01-0.482D-01-0.185D+00-0.214D+00 0.466D+00

Coeff: 0.925D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=2.15D-07 MaxDP=1.05D-05 DE=-6.11D-09 OVMax= 1.58D-04

Cycle 14 Pass 1 IDiag 1:

RMSU= 3.17D-08 CP: 1.00D+00 1.13D+00 6.32D-01 1.39D+00 1.88D+00

CP: 2.39D+00 2.28D+00 1.96D+00 2.50D+00 2.56D+00

CP: 2.78D+00 2.04D+00 1.30D+00

E= -1275.84160512506 Delta-E= -0.000000002738 Rises=F Damp=F

DIIS: error= 8.53D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84160512506 IErMin=14 ErrMin= 8.53D-07

ErrMax= 8.53D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.63D-10 BMatP= 1.29D-09

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

Coeff-Com: -0.157D-04 0.726D-03 0.594D-03 0.138D-03-0.449D-02-0.150D-01

Coeff-Com: 0.113D-01 0.456D-01 0.486D-01-0.518D-01-0.394D+00-0.460D-01

Coeff-Com: 0.565D+00 0.839D+00

Coeff: -0.157D-04 0.726D-03 0.594D-03 0.138D-03-0.449D-02-0.150D-01

Coeff: 0.113D-01 0.456D-01 0.486D-01-0.518D-01-0.394D+00-0.460D-01

Coeff: 0.565D+00 0.839D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=1.60D-07 MaxDP=8.21D-06 DE=-2.74D-09 OVMax= 1.18D-04

Cycle 15 Pass 1 IDiag 1:

RMSU= 3.12D-08 CP: 1.00D+00 1.13D+00 6.32D-01 1.40D+00 1.89D+00

CP: 2.41D+00 2.31D+00 2.02D+00 2.64D+00 2.76D+00

CP: 3.00D+00 2.51D+00 1.84D+00 1.18D+00

E= -1275.84160512595 Delta-E= -0.000000000888 Rises=F Damp=F

DIIS: error= 3.00D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.84160512595 IErMin=15 ErrMin= 3.00D-07

ErrMax= 3.00D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.07D-10 BMatP= 4.63D-10

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

Coeff-Com: -0.228D-04 0.545D-03 0.755D-03 0.117D-02-0.139D-02-0.843D-02

Coeff-Com: -0.109D-02 0.168D-01 0.376D-01 0.178D-01-0.159D+00-0.123D+00

Coeff-Com: 0.665D-01 0.447D+00 0.704D+00

Coeff: -0.228D-04 0.545D-03 0.755D-03 0.117D-02-0.139D-02-0.843D-02

Coeff: -0.109D-02 0.168D-01 0.376D-01 0.178D-01-0.159D+00-0.123D+00

Coeff: 0.665D-01 0.447D+00 0.704D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=4.22D-08 MaxDP=1.78D-06 DE=-8.88D-10 OVMax= 2.87D-05

Cycle 16 Pass 1 IDiag 1:

RMSU= 1.23D-08 CP: 1.00D+00 1.13D+00 6.32D-01 1.40D+00 1.89D+00

CP: 2.42D+00 2.32D+00 2.03D+00 2.67D+00 2.81D+00

CP: 3.00D+00 2.66D+00 2.02D+00 1.43D+00 1.47D+00

E= -1275.84160512608 Delta-E= -0.000000000133 Rises=F Damp=F

DIIS: error= 1.39D-07 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1275.84160512608 IErMin=16 ErrMin= 1.39D-07

ErrMax= 1.39D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.28D-11 BMatP= 1.07D-10

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

Coeff-Com: -0.403D-05-0.131D-04 0.126D-03 0.448D-03 0.986D-03 0.139D-02

Coeff-Com: -0.387D-02-0.816D-02-0.949D-03 0.242D-01 0.572D-01-0.324D-01

Coeff-Com: -0.161D+00-0.844D-01 0.300D+00 0.906D+00

Coeff: -0.403D-05-0.131D-04 0.126D-03 0.448D-03 0.986D-03 0.139D-02

Coeff: -0.387D-02-0.816D-02-0.949D-03 0.242D-01 0.572D-01-0.324D-01

Coeff: -0.161D+00-0.844D-01 0.300D+00 0.906D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=2.24D-08 MaxDP=1.08D-06 DE=-1.33D-10 OVMax= 1.38D-05

Cycle 17 Pass 1 IDiag 1:

RMSU= 3.80D-09 CP: 1.00D+00 1.13D+00 6.32D-01 1.40D+00 1.89D+00

CP: 2.42D+00 2.32D+00 2.04D+00 2.69D+00 2.85D+00

CP: 3.00D+00 2.74D+00 2.11D+00 1.58D+00 1.83D+00

CP: 1.06D+00

E= -1275.84160512610 Delta-E= -0.000000000020 Rises=F Damp=F

DIIS: error= 8.28D-08 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=17 EnMin= -1275.84160512610 IErMin=17 ErrMin= 8.28D-08

ErrMax= 8.28D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.08D-12 BMatP= 2.28D-11

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

Coeff-Com: 0.131D-05-0.976D-04-0.628D-04 0.594D-04 0.760D-03 0.202D-02

Coeff-Com: -0.200D-02-0.742D-02-0.689D-02 0.111D-01 0.594D-01 0.277D-02

Coeff-Com: -0.107D+00-0.120D+00 0.552D-01 0.541D+00 0.571D+00

Coeff: 0.131D-05-0.976D-04-0.628D-04 0.594D-04 0.760D-03 0.202D-02

Coeff: -0.200D-02-0.742D-02-0.689D-02 0.111D-01 0.594D-01 0.277D-02

Coeff: -0.107D+00-0.120D+00 0.552D-01 0.541D+00 0.571D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=5.52D-09 MaxDP=2.65D-07 DE=-1.96D-11 OVMax= 3.36D-06

Error on total polarization charges = 0.06498

SCF Done: E(UB3LYP) = -1275.84160513 A.U. after 17 cycles

NFock= 17 Conv=0.55D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0187 S= 1.0062

<L.S>= 0.000000000000E+00

KE= 1.320693300804D+03 PE=-8.570112154273D+03 EE= 3.214515233763D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.72

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0187, after 2.0002

Leave Link 502 at Tue Sep 17 14:03:44 2019, MaxMem= 2415919104 cpu: 1641.0

(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= 15317 LenP2D= 41236.

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 = 256

Leave Link 701 at Tue Sep 17 14:03:48 2019, MaxMem= 2415919104 cpu: 74.1

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 14:03:48 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 14:04:00 2019, MaxMem= 2415919104 cpu: 212.6

(Enter /home/blab/g09/l716.exe)

Dipole = 4.31654712D-13-3.48165941D-13 0.00000000D+00

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.005682714 0.008662717 0.000000000

2 7 -0.004776386 0.002322304 -0.000000000

3 6 0.009703978 0.003359193 0.000000000

4 6 -0.009276894 0.003010775 0.000000000

5 6 0.002580389 -0.009678857 0.000000000

6 7 -0.007329688 -0.007680831 -0.000000000

7 6 0.002100321 0.000657056 -0.000000000

8 7 0.002832428 0.004114272 -0.000000000

9 6 -0.009094427 -0.006034198 -0.000000000

10 6 0.002944714 -0.003961841 -0.000000000

11 6 -0.000229002 0.005723302 -0.000000000

12 7 -0.007206549 -0.011819170 -0.000000000

13 6 -0.002944714 0.003961841 -0.000000000

14 6 0.000229002 -0.005723302 0.000000000

15 6 -0.002100321 -0.000657056 0.000000000

16 7 -0.002832428 -0.004114272 -0.000000000

17 6 0.009094427 0.006034198 0.000000000

18 7 0.007329688 0.007680831 -0.000000000

19 7 0.004776386 -0.002322304 -0.000000000

20 6 -0.009703978 -0.003359193 0.000000000

21 6 0.009276894 -0.003010775 -0.000000000

22 6 -0.002580389 0.009678857 -0.000000000

23 6 -0.005682714 -0.008662717 -0.000000000

24 7 0.007206549 0.011819170 -0.000000000

25 30 0.000000000 -0.000000000 0.000000000

26 6 0.000562818 -0.000201974 0.000000000

27 1 0.001592652 0.000474538 0.000000000

28 6 -0.001276075 -0.000009943 -0.000000000

29 1 -0.000402239 0.000765040 -0.000000000

30 6 0.001276075 0.000009943 -0.000000000

31 1 0.000402239 -0.000765040 -0.000000000

32 6 -0.000562818 0.000201974 -0.000000000

33 1 -0.001592652 -0.000474538 0.000000000

34 1 0.001382160 0.000855072 -0.000000000

35 1 -0.001148665 0.000417920 -0.003559799

36 1 -0.001148665 0.000417920 0.003559799

37 1 -0.000365836 -0.001167331 -0.003663115

38 1 -0.000365836 -0.001167331 0.003663115

39 1 -0.000708976 0.001534021 -0.000000000

40 1 0.000365836 0.001167331 -0.003663115

41 1 0.000365836 0.001167331 0.003663115

42 1 0.000708976 -0.001534021 -0.000000000

43 1 0.001148665 -0.000417920 -0.003559799

44 1 0.001148665 -0.000417920 0.003559799

45 1 -0.001382160 -0.000855072 -0.000000000

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

Cartesian Forces: Max 0.011819170 RMS 0.003879765

Leave Link 716 at Tue Sep 17 14:04:00 2019, MaxMem= 2415919104 cpu: 0.4

(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 0.008276414 RMS 0.001813216

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= -6.41D-03 DEPred=-7.05D-03 R= 9.09D-01

TightC=F SS= 1.41D+00 RLast= 1.50D-01 DXNew= 2.5227D-01 4.5109D-01

Trust test= 9.09D-01 RLast= 1.50D-01 DXMaxT set to 2.52D-01

ITU= 1 -1 1 1 1 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01332

Eigenvalues --- 0.01333 0.01344 0.01345 0.01603 0.01624

Eigenvalues --- 0.01631 0.01642 0.01771 0.01791 0.01806

Eigenvalues --- 0.01820 0.01883 0.01903 0.01933 0.01947

Eigenvalues --- 0.01997 0.01999 0.02042 0.02048 0.02070

Eigenvalues --- 0.02086 0.02102 0.02109 0.02114 0.02205

Eigenvalues --- 0.02314 0.02321 0.02354 0.02375 0.07211

Eigenvalues --- 0.07263 0.07263 0.07300 0.07300 0.07325

Eigenvalues --- 0.07395 0.07443 0.13144 0.14479 0.14514

Eigenvalues --- 0.15489 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16012 0.16024 0.16134

Eigenvalues --- 0.16299 0.16559 0.18324 0.20649 0.22068

Eigenvalues --- 0.22113 0.23849 0.23852 0.23895 0.24355

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25007 0.25037 0.25248

Eigenvalues --- 0.28812 0.30912 0.32370 0.33192 0.33200

Eigenvalues --- 0.33282 0.33282 0.33338 0.33519 0.33684

Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33729 0.34378 0.34437 0.34437

Eigenvalues --- 0.34439 0.35325 0.35556 0.35571 0.35596

Eigenvalues --- 0.35682 0.35682 0.35754 0.37805 0.38569

Eigenvalues --- 0.40318 0.41630 0.41855 0.43967 0.48022

Eigenvalues --- 0.48946 0.49008 0.49159 0.51135 0.51349

Eigenvalues --- 0.51370 0.53903 0.53950 0.54022 0.55367

Eigenvalues --- 0.56318 0.56368 0.57190 0.93922

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 0.63954 -0.16682 0.52728

Cosine: 0.953 > 0.840

Length: 1.243

GDIIS step was calculated using 3 of the last 8 vectors.

Iteration 1 RMS(Cart)= 0.00769769 RMS(Int)= 0.00003391

Iteration 2 RMS(Cart)= 0.00004828 RMS(Int)= 0.00000979

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000979

ITry= 1 IFail=0 DXMaxC= 3.13D-02 DCOld= 1.00D+10 DXMaxT= 2.52D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 2.27D-09 for atom 36.

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

(Linear) (Quad) (Total)

R1 2.60260 -0.00134 0.01085 -0.00852 0.00234 2.60494

R2 2.70932 0.00425 0.01715 0.00221 0.01936 2.72868

R3 2.58391 -0.00205 -0.02617 0.00359 -0.02257 2.56134

R4 2.54744 0.00103 -0.00848 0.00806 -0.00043 2.54701

R5 3.80720 -0.00165 -0.00679 -0.00416 -0.01093 3.79627

R6 2.76877 0.00226 0.02604 -0.00695 0.01910 2.78787

R7 2.59435 -0.00448 -0.01945 -0.00227 -0.02174 2.57261

R8 2.62056 -0.00828 -0.02021 -0.00064 -0.02084 2.59972

R9 2.81591 -0.00152 -0.00414 0.00093 -0.00321 2.81269

R10 2.04775 -0.00162 -0.00180 -0.00083 -0.00263 2.04512

R11 2.48930 0.00572 0.02959 -0.00499 0.02458 2.51389

R12 2.56701 0.00188 -0.01209 0.00807 -0.00401 2.56300

R13 2.80986 -0.00130 -0.01012 -0.00294 -0.01306 2.79679

R14 2.59759 -0.00207 0.00725 -0.00678 0.00046 2.59805

R15 3.78658 -0.00231 0.00162 -0.00496 -0.00333 3.78325

R16 2.83042 0.00085 -0.01740 0.00260 -0.01480 2.81562

R17 2.46641 0.00726 0.02114 0.00139 0.02252 2.48893

R18 2.55873 -0.00420 0.00541 -0.00166 0.00375 2.56248

R19 2.81858 -0.00283 -0.00265 -0.00148 -0.00413 2.81445

R20 2.04514 -0.00087 -0.00100 -0.00028 -0.00128 2.04386

R21 2.46641 0.00726 0.02114 0.00139 0.02252 2.48893

R22 2.55873 -0.00420 0.00541 -0.00166 0.00375 2.56248

R23 2.83042 0.00085 -0.01740 0.00260 -0.01480 2.81562

R24 2.81858 -0.00283 -0.00265 -0.00148 -0.00413 2.81445

R25 2.80986 -0.00130 -0.01012 -0.00294 -0.01306 2.79679

R26 2.04514 -0.00087 -0.00100 -0.00028 -0.00128 2.04386

R27 2.56701 0.00188 -0.01209 0.00807 -0.00401 2.56300

R28 2.48930 0.00572 0.02959 -0.00499 0.02458 2.51389

R29 2.59759 -0.00207 0.00725 -0.00678 0.00046 2.59805

R30 3.78658 -0.00231 0.00162 -0.00496 -0.00333 3.78325

R31 2.59435 -0.00448 -0.01945 -0.00227 -0.02174 2.57261

R32 2.54744 0.00103 -0.00848 0.00806 -0.00043 2.54701

R33 2.60260 -0.00134 0.01085 -0.00852 0.00234 2.60494

R34 3.80720 -0.00165 -0.00679 -0.00416 -0.01093 3.79627

R35 2.76877 0.00226 0.02604 -0.00695 0.01910 2.78787

R36 2.62056 -0.00828 -0.02021 -0.00064 -0.02084 2.59972

R37 2.81591 -0.00152 -0.00414 0.00093 -0.00321 2.81269

R38 2.70932 0.00425 0.01715 0.00221 0.01936 2.72868

R39 2.04775 -0.00162 -0.00180 -0.00083 -0.00263 2.04512

R40 2.58391 -0.00205 -0.02617 0.00359 -0.02257 2.56134

R41 2.06713 -0.00162 -0.00218 -0.00059 -0.00277 2.06436

R42 2.07997 -0.00359 -0.00430 -0.00160 -0.00590 2.07407

R43 2.07997 -0.00359 -0.00430 -0.00160 -0.00590 2.07407

R44 2.07889 -0.00367 -0.00437 -0.00156 -0.00593 2.07296

R45 2.07889 -0.00367 -0.00437 -0.00156 -0.00593 2.07296

R46 2.06650 -0.00164 -0.00202 -0.00061 -0.00263 2.06387

R47 2.07889 -0.00367 -0.00437 -0.00156 -0.00593 2.07296

R48 2.07889 -0.00367 -0.00437 -0.00156 -0.00593 2.07296

R49 2.06650 -0.00164 -0.00202 -0.00061 -0.00263 2.06387

R50 2.07997 -0.00359 -0.00430 -0.00160 -0.00590 2.07407

R51 2.07997 -0.00359 -0.00430 -0.00160 -0.00590 2.07407

R52 2.06713 -0.00162 -0.00218 -0.00059 -0.00277 2.06436

A1 1.88976 0.00081 -0.00343 0.00245 -0.00101 1.88876

A2 2.19068 0.00233 0.00696 0.00257 0.00957 2.20025

A3 2.20274 -0.00314 -0.00353 -0.00502 -0.00856 2.19418

A4 1.90463 -0.00095 0.00393 -0.00175 0.00215 1.90679

A5 2.17382 0.00231 0.00339 0.00288 0.00631 2.18012

A6 2.20474 -0.00136 -0.00732 -0.00113 -0.00846 2.19628

A7 1.90507 -0.00161 -0.00634 -0.00025 -0.00656 1.89851

A8 2.20928 0.00306 0.01691 -0.00248 0.01441 2.22369

A9 2.16884 -0.00145 -0.01057 0.00272 -0.00785 2.16099

A10 1.84089 0.00297 0.00607 0.00163 0.00771 1.84859

A11 2.18301 -0.00180 -0.01196 0.00236 -0.00961 2.17341

A12 2.25929 -0.00117 0.00589 -0.00399 0.00190 2.26119

A13 1.88443 -0.00121 -0.00023 -0.00207 -0.00230 1.88213

A14 2.17902 0.00101 -0.00295 0.00230 -0.00065 2.17837

A15 2.21973 0.00021 0.00318 -0.00022 0.00295 2.22268

A16 2.16740 -0.00279 -0.01073 0.00351 -0.00726 2.16015

A17 2.22991 0.00105 -0.00052 -0.00071 -0.00123 2.22869

A18 2.16264 0.00104 0.00044 0.00204 0.00248 2.16512

A19 1.89063 -0.00209 0.00008 -0.00133 -0.00125 1.88938

A20 1.91049 0.00101 0.00008 -0.00039 -0.00031 1.91018

A21 2.20407 -0.00155 -0.00210 -0.00200 -0.00406 2.20001

A22 2.16862 0.00054 0.00202 0.00239 0.00437 2.17299

A23 1.88530 -0.00103 0.00023 0.00090 0.00114 1.88644

A24 2.22877 0.00332 -0.00158 0.00332 0.00173 2.23050

A25 2.16912 -0.00229 0.00135 -0.00422 -0.00287 2.16625

A26 1.85898 0.00026 -0.00195 -0.00015 -0.00210 1.85688

A27 2.15800 -0.00064 0.00391 0.00059 0.00450 2.16250

A28 2.26621 0.00038 -0.00197 -0.00044 -0.00241 2.26380

A29 1.87938 0.00185 0.00155 0.00097 0.00252 1.88190

A30 2.16794 -0.00089 0.00109 0.00043 0.00153 2.16947

A31 2.23587 -0.00096 -0.00265 -0.00141 -0.00405 2.23182

A32 2.21386 -0.00692 -0.00703 -0.00836 -0.01538 2.19848

A33 1.85898 0.00026 -0.00195 -0.00015 -0.00210 1.85688

A34 2.26621 0.00038 -0.00197 -0.00044 -0.00241 2.26380

A35 2.15800 -0.00064 0.00391 0.00059 0.00450 2.16250

A36 1.87938 0.00185 0.00155 0.00097 0.00252 1.88190

A37 2.23587 -0.00096 -0.00265 -0.00141 -0.00405 2.23182

A38 2.16794 -0.00089 0.00109 0.00043 0.00153 2.16947

A39 1.89063 -0.00209 0.00008 -0.00133 -0.00125 1.88938

A40 2.16264 0.00104 0.00044 0.00204 0.00248 2.16512

A41 2.22991 0.00105 -0.00052 -0.00071 -0.00123 2.22869

A42 1.91049 0.00101 0.00008 -0.00039 -0.00031 1.91018

A43 2.20407 -0.00155 -0.00210 -0.00200 -0.00406 2.20001

A44 2.16862 0.00054 0.00202 0.00239 0.00437 2.17299

A45 2.16912 -0.00229 0.00135 -0.00422 -0.00287 2.16625

A46 2.22877 0.00332 -0.00158 0.00332 0.00173 2.23050

A47 1.88530 -0.00103 0.00023 0.00090 0.00114 1.88644

A48 2.16740 -0.00279 -0.01073 0.00351 -0.00726 2.16015

A49 1.90463 -0.00095 0.00393 -0.00175 0.00215 1.90679

A50 2.20474 -0.00136 -0.00732 -0.00113 -0.00846 2.19628

A51 2.17382 0.00231 0.00339 0.00288 0.00631 2.18012

A52 2.20928 0.00306 0.01691 -0.00248 0.01441 2.22369

A53 2.16884 -0.00145 -0.01057 0.00272 -0.00785 2.16099

A54 1.90507 -0.00161 -0.00634 -0.00025 -0.00656 1.89851

A55 1.84089 0.00297 0.00607 0.00163 0.00771 1.84859

A56 2.18301 -0.00180 -0.01196 0.00236 -0.00961 2.17341

A57 2.25929 -0.00117 0.00589 -0.00399 0.00190 2.26119

A58 1.88443 -0.00121 -0.00023 -0.00207 -0.00230 1.88213

A59 2.21973 0.00021 0.00318 -0.00022 0.00295 2.22268

A60 2.17902 0.00101 -0.00295 0.00230 -0.00065 2.17837

A61 1.88976 0.00081 -0.00343 0.00245 -0.00101 1.88876

A62 2.19068 0.00233 0.00696 0.00257 0.00957 2.20025

A63 2.20274 -0.00314 -0.00353 -0.00502 -0.00856 2.19418

A64 2.21386 -0.00692 -0.00703 -0.00836 -0.01538 2.19848

A65 1.55097 0.00159 0.00377 0.00280 0.00659 1.55756

A66 1.59063 -0.00159 -0.00377 -0.00280 -0.00659 1.58403

A67 1.59063 -0.00159 -0.00377 -0.00280 -0.00659 1.58403

A68 1.55097 0.00159 0.00377 0.00280 0.00659 1.55756

A69 1.93907 0.00028 0.00371 -0.00079 0.00292 1.94200

A70 1.93732 0.00054 -0.00032 0.00075 0.00043 1.93775

A71 1.93732 0.00054 -0.00032 0.00075 0.00043 1.93775

A72 1.88787 -0.00008 0.00226 -0.00028 0.00199 1.88987

A73 1.88787 -0.00008 0.00226 -0.00028 0.00199 1.88987

A74 1.87197 -0.00128 -0.00792 -0.00017 -0.00808 1.86389

A75 1.93120 0.00051 0.00295 -0.00028 0.00267 1.93387

A76 1.93120 0.00051 0.00295 -0.00028 0.00267 1.93387

A77 1.93690 0.00064 0.00309 0.00045 0.00354 1.94044

A78 1.87555 -0.00135 -0.00774 -0.00075 -0.00849 1.86706

A79 1.89364 -0.00020 -0.00088 0.00042 -0.00046 1.89319

A80 1.89364 -0.00020 -0.00088 0.00042 -0.00046 1.89319

A81 1.93120 0.00051 0.00295 -0.00028 0.00267 1.93387

A82 1.93120 0.00051 0.00295 -0.00028 0.00267 1.93387

A83 1.93690 0.00064 0.00309 0.00045 0.00354 1.94044

A84 1.87555 -0.00135 -0.00774 -0.00075 -0.00849 1.86706

A85 1.89364 -0.00020 -0.00088 0.00042 -0.00046 1.89319

A86 1.89364 -0.00020 -0.00088 0.00042 -0.00046 1.89319

A87 1.93732 0.00054 -0.00032 0.00075 0.00043 1.93775

A88 1.93732 0.00054 -0.00032 0.00075 0.00043 1.93775

A89 1.93907 0.00028 0.00371 -0.00079 0.00292 1.94200

A90 1.87197 -0.00128 -0.00792 -0.00017 -0.00808 1.86389

A91 1.88787 -0.00008 0.00226 -0.00028 0.00199 1.88987

A92 1.88787 -0.00008 0.00226 -0.00028 0.00199 1.88987

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 1.04013 -0.00045 -0.00516 0.00038 -0.00479 1.03535

D31 -1.04013 0.00045 0.00516 -0.00038 0.00479 -1.03535

D32 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.10146 -0.00045 -0.00516 0.00038 -0.00479 -2.10625

D34 2.10146 0.00045 0.00516 -0.00038 0.00479 2.10625

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 1.03840 -0.00051 -0.00294 -0.00064 -0.00358 1.03482

D64 -1.03840 0.00051 0.00294 0.00064 0.00358 -1.03482

D65 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D66 -2.10319 -0.00051 -0.00294 -0.00064 -0.00358 -2.10677

D67 2.10319 0.00051 0.00294 0.00064 0.00358 2.10677

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 -2.10319 -0.00051 -0.00294 -0.00064 -0.00358 -2.10677

D80 2.10319 0.00051 0.00294 0.00064 0.00358 2.10677

D81 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D82 1.03840 -0.00051 -0.00294 -0.00064 -0.00358 1.03482

D83 -1.03840 0.00051 0.00294 0.00064 0.00358 -1.03482

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 1.04013 -0.00045 -0.00516 0.00038 -0.00479 1.03535

D126 -1.04013 0.00045 0.00516 -0.00038 0.00479 -1.03535

D127 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D128 -2.10146 -0.00045 -0.00516 0.00038 -0.00479 -2.10625

D129 2.10146 0.00045 0.00516 -0.00038 0.00479 2.10625

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 0.008276 0.000450 NO

RMS Force 0.001813 0.000300 NO

Maximum Displacement 0.031346 0.001800 NO

RMS Displacement 0.007712 0.001200 NO

Predicted change in Energy=-8.774379D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:04:00 2019, MaxMem= 2415919104 cpu: 1.7

(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 -2.072538 -2.193212 0.000000

2 7 0 -0.732330 -1.870659 0.000000

3 6 0 -0.002539 -3.003807 0.000000

4 6 0 -0.919717 -4.159328 0.000000

5 6 0 -2.190490 -3.632342 0.000000

6 7 0 1.354394 -3.113572 0.000000

7 6 0 2.180554 -2.070915 0.000000

8 7 0 1.854422 -0.754429 0.000000

9 6 0 3.002740 0.001563 0.000000

10 6 0 4.167886 -0.927102 0.000000

11 6 0 3.656310 -2.182904 0.000000

12 7 0 -3.104684 -1.314699 0.000000

13 6 0 -4.167886 0.927102 0.000000

14 6 0 -3.656310 2.182904 0.000000

15 6 0 -2.180554 2.070915 0.000000

16 7 0 -1.854422 0.754429 0.000000

17 6 0 -3.002740 -0.001563 0.000000

18 7 0 -1.354394 3.113572 0.000000

19 7 0 0.732330 1.870659 0.000000

20 6 0 0.002539 3.003807 0.000000

21 6 0 0.919717 4.159328 0.000000

22 6 0 2.190490 3.632342 0.000000

23 6 0 2.072538 2.193212 0.000000

24 7 0 3.104684 1.314699 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.483733 -5.582455 0.000000

27 1 0 -3.126538 -4.175517 0.000000

28 6 0 5.587972 -0.478213 0.000000

29 1 0 4.196467 -3.119925 0.000000

30 6 0 -5.587972 0.478213 0.000000

31 1 0 -4.196467 3.119925 0.000000

32 6 0 0.483733 5.582455 0.000000

33 1 0 3.126538 4.175517 0.000000

34 1 0 -1.341021 -6.259524 0.000000

35 1 0 0.131401 -5.805842 0.881091

36 1 0 0.131401 -5.805842 -0.881091

37 1 0 5.801602 0.138532 0.881658

38 1 0 5.801602 0.138532 -0.881658

39 1 0 6.271142 -1.330315 0.000000

40 1 0 -5.801602 -0.138532 0.881658

41 1 0 -5.801602 -0.138532 -0.881658

42 1 0 -6.271142 1.330315 0.000000

43 1 0 -0.131401 5.805842 0.881091

44 1 0 -0.131401 5.805842 -0.881091

45 1 0 1.341021 6.259524 0.000000

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Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.378476 0.000000

3 C 2.223051 1.347820 0.000000

4 C 2.279168 2.296327 1.475277 0.000000

5 C 1.443955 2.286866 2.276442 1.375711 0.000000

6 N 3.548369 2.428838 1.361366 2.503035 3.582643

7 C 4.254850 2.919760 2.374065 3.738067 4.641561

8 N 4.182237 2.817314 2.916849 4.391945 4.964242

9 C 5.529510 4.178034 4.250171 5.718276 6.338368

10 C 6.367568 4.990232 4.658878 6.027518 6.909940

11 C 5.728856 4.399734 3.749808 4.984603 6.023781

12 N 1.355401 2.436628 3.532194 3.586920 2.491429

13 C 3.758569 4.430633 5.727316 6.035094 4.969770

14 C 4.653894 4.998102 6.344447 6.907448 5.997142

15 C 4.265495 4.199210 5.522369 6.356543 5.703266

16 N 2.955700 2.854851 4.189726 5.001867 4.399625

17 C 2.380883 2.940796 4.244370 4.650376 3.720525

18 N 5.355156 5.022900 6.264969 7.285878 6.797530

19 N 4.937847 4.017797 4.929549 6.252200 6.231044

20 C 5.595977 4.929549 6.007616 7.222261 6.989124

21 C 7.021990 6.252200 7.222261 8.519597 8.389488

22 C 7.218760 6.231044 6.989124 8.389488 8.483433

23 C 6.035095 4.937847 5.595977 7.021990 7.218760

24 N 6.253725 4.986902 5.320182 6.794172 7.246523

25 Zn 3.017547 2.008899 3.003808 4.259799 4.241716

26 C 3.743163 3.720112 2.623161 1.488414 2.591518

27 H 2.245094 3.323342 3.336506 2.206881 1.082231

28 C 7.850135 6.471872 6.134528 7.476671 8.393628

29 H 6.337130 5.084655 4.200612 5.220699 6.407480

30 C 4.415291 5.393927 6.581909 6.580227 5.332874

31 H 5.721932 6.075045 7.422205 7.982770 7.043937

32 C 8.185079 7.551670 8.600021 9.842358 9.594997

33 H 8.221381 7.172664 7.831591 9.265085 9.446346

34 H 4.131587 4.430873 3.520117 2.142037 2.761102

35 H 4.322587 4.124077 2.940350 2.142937 3.300243

36 H 4.322587 4.124077 2.940350 2.142937 3.300243

37 H 8.259324 6.892492 6.658804 8.026521 8.880898

38 H 8.259324 6.892492 6.658804 8.026521 8.880898

39 H 8.388181 7.024286 6.493046 7.727338 8.769182

40 H 4.347983 5.429098 6.528112 6.385681 5.101388

41 H 4.347983 5.429098 6.528112 6.385681 5.101388

42 H 5.481198 6.397239 7.621023 7.666416 6.424927

43 H 8.278236 7.750232 8.854538 10.035056 9.700282

44 H 8.278236 7.750232 8.854538 10.035056 9.700282

45 H 9.115982 8.390391 9.360259 10.661304 10.503361

6 7 8 9 10

6 N 0.000000

7 C 1.330291 0.000000

8 N 2.411553 1.356281 0.000000

9 C 3.524360 2.229609 1.374830 0.000000

10 C 3.563199 2.292988 2.319899 1.489960 0.000000

11 C 2.482933 1.479998 2.299422 2.280142 1.356005

12 N 4.808256 5.339065 4.990655 6.247654 7.282891

13 C 6.842706 7.020740 6.252658 7.230110 8.539505

14 C 7.291078 7.222462 6.244684 7.007224 8.419630

15 C 6.274932 6.014485 4.925810 5.581107 7.020740

16 N 5.025727 4.925810 4.004019 4.915163 6.252658

17 C 5.354365 5.581107 4.915163 6.005481 7.230110

18 N 6.790793 6.274932 5.025727 5.354365 6.842706

19 N 5.022900 4.199210 2.854851 2.940796 4.430633

20 C 6.264969 5.522369 4.189726 4.244370 5.727316

21 C 7.285878 6.356543 5.001867 4.650376 6.035094

22 C 6.797530 5.703266 4.399625 3.720525 4.969770

23 C 5.355156 4.265495 2.955700 2.380883 3.758569

24 N 4.761628 3.509473 2.417529 1.317087 2.481142

25 Zn 3.395396 3.007242 2.002010 3.002741 4.269753

26 C 3.078002 4.407872 5.364402 6.583066 6.581023

27 H 4.605050 5.709166 6.042666 7.417280 7.985037

28 C 4.986812 3.761275 3.743753 2.629374 1.489344

29 H 2.842080 2.272516 3.328776 3.341956 2.193010

30 C 7.816481 8.176066 7.543781 8.603925 9.856554

31 H 8.346769 8.222605 7.184976 7.845557 9.291976

32 C 8.739505 7.839215 6.483432 6.123051 7.479794

33 H 7.501421 6.317658 5.091428 4.175789 5.207794

34 H 4.142738 5.472288 6.365291 7.620333 7.666993

35 H 3.085506 4.350290 5.409426 6.538108 6.393092

36 H 3.085506 4.350290 5.409426 6.538108 6.393092

37 H 5.579530 4.332547 4.141851 2.937637 2.140543

38 H 5.579530 4.332547 4.141851 2.937637 2.140543

39 H 5.230145 4.157090 4.454106 3.529356 2.141558

40 H 7.799774 8.259918 7.731193 8.849485 10.039415

41 H 7.799774 8.259918 7.731193 8.849485 10.039415

42 H 8.825925 9.110408 8.388739 9.368590 10.680320

43 H 9.085145 8.256195 6.910641 6.654984 8.036959

44 H 9.085145 8.256195 6.910641 6.654984 8.036959

45 H 9.373106 8.372636 7.032717 6.474827 7.722613

11 12 13 14 15

11 C 0.000000

12 N 6.816511 0.000000

13 C 8.419630 2.481142 0.000000

14 C 8.516729 3.540836 1.356005 0.000000

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16 N 6.244684 2.417529 2.319899 2.299422 1.356281

17 C 7.007224 1.317087 1.489960 2.280142 2.229609

18 N 7.291078 4.761628 3.563199 2.482933 1.330291

19 N 4.998102 4.986902 4.990232 4.399734 2.919760

20 C 6.344447 5.320182 4.658878 3.749808 2.374065

21 C 6.907448 6.794172 6.027518 4.984603 3.738067

22 C 5.997142 7.246523 6.909940 6.023781 4.641561

23 C 4.653894 6.253725 6.367568 5.728856 4.254850

24 N 3.540836 6.743144 7.282891 6.816511 5.339065

25 Zn 4.258365 3.371572 4.269753 4.258365 3.007242

26 C 5.356949 5.008306 7.479794 8.388447 7.839215

27 H 7.069479 2.860901 5.207794 6.380452 6.317658

28 C 2.576293 8.732810 9.856554 9.619682 8.176066

29 H 1.081563 7.521014 9.291976 9.475553 8.222605

30 C 9.619682 3.062883 1.489344 2.576293 3.761275

31 H 9.475553 4.567043 2.193010 1.081563 2.272516

32 C 8.388447 7.774797 6.581023 5.356949 4.407872

33 H 6.380452 8.304854 7.985037 7.069479 5.709166

34 H 6.449197 5.249934 7.722613 8.754151 8.372636

35 H 5.130982 5.605260 8.036959 8.884995 8.256195

36 H 5.130982 5.605260 8.036959 8.884995 8.256195

37 H 3.281564 9.067036 10.039415 9.716423 8.259918

38 H 3.281564 9.067036 10.039415 9.716423 8.259918

39 H 2.750319 9.375840 10.680320 10.530765 9.110408

40 H 9.716423 3.071490 2.140543 3.281564 4.332547

41 H 9.716423 3.071490 2.140543 3.281564 4.332547

42 H 10.530765 4.125840 2.141558 2.750319 4.157090

43 H 8.884995 7.766520 6.393092 5.130982 4.350290

44 H 8.884995 7.766520 6.393092 5.130982 4.350290

45 H 8.754151 8.782548 7.666993 6.449197 5.472288

16 17 18 19 20

16 N 0.000000

17 C 1.374830 0.000000

18 N 2.411553 3.524360 0.000000

19 N 2.817314 4.178034 2.428838 0.000000

20 C 2.916849 4.250171 1.361366 1.347820 0.000000

21 C 4.391945 5.718276 2.503035 2.296327 1.475277

22 C 4.964242 6.338368 3.582643 2.286866 2.276442

23 C 4.182237 5.529510 3.548369 1.378476 2.223051

24 N 4.990655 6.247654 4.808256 2.436628 3.532194

25 Zn 2.002010 3.002741 3.395396 2.008899 3.003808

26 C 6.483432 6.123051 8.739505 7.551670 8.600021

27 H 5.091428 4.175789 7.501421 7.172664 7.831591

28 C 7.543781 8.603925 7.816481 5.393927 6.581909

29 H 7.184976 7.845557 8.346769 6.075045 7.422205

30 C 3.743753 2.629374 4.986812 6.471872 6.134528

31 H 3.328776 3.341956 2.842080 5.084655 4.200612

32 C 5.364402 6.583066 3.078002 3.720112 2.623161

33 H 6.042666 7.417280 4.605050 3.323342 3.336506

34 H 7.032717 6.474827 9.373106 8.390391 9.360259

35 H 6.910641 6.654984 9.085145 7.750232 8.854538

36 H 6.910641 6.654984 9.085145 7.750232 8.854538

37 H 7.731193 8.849485 7.799774 5.429098 6.528112

38 H 7.731193 8.849485 7.799774 5.429098 6.528112

39 H 8.388739 9.368590 8.825925 6.397239 7.621023

40 H 4.141851 2.937637 5.579530 6.892492 6.658804

41 H 4.141851 2.937637 5.579530 6.892492 6.658804

42 H 4.454106 3.529356 5.230145 7.024286 6.493046

43 H 5.409426 6.538108 3.085506 4.124077 2.940350

44 H 5.409426 6.538108 3.085506 4.124077 2.940350

45 H 6.365291 7.620333 4.142738 4.430873 3.520117

21 22 23 24 25

21 C 0.000000

22 C 1.375711 0.000000

23 C 2.279168 1.443955 0.000000

24 N 3.586920 2.491429 1.355401 0.000000

25 Zn 4.259799 4.241716 3.017547 3.371572 0.000000

26 C 9.842358 9.594997 8.185079 7.774797 5.603374

27 H 9.265085 9.446346 8.221381 8.304854 5.216338

28 C 6.580227 5.332874 4.415291 3.062883 5.608397

29 H 7.982770 7.043937 5.721932 4.567043 5.229175

30 C 7.476671 8.393628 7.850135 8.732810 5.608397

31 H 5.220699 6.407480 6.337130 7.521014 5.229175

32 C 1.488414 2.591518 3.743163 5.008306 5.603374

33 H 2.206881 1.082231 2.245094 2.860901 5.216338

34 H 10.661304 10.503361 9.115982 8.782548 6.401561

35 H 10.035056 9.700282 8.278236 7.766520 5.873788

36 H 10.035056 9.700282 8.278236 7.766520 5.873788

37 H 6.385681 5.101388 4.347983 3.071490 5.869847

38 H 6.385681 5.101388 4.347983 3.071490 5.869847

39 H 7.666416 6.424927 5.481198 4.125840 6.410691

40 H 8.026521 8.880898 8.259324 9.067036 5.869847

41 H 8.026521 8.880898 8.259324 9.067036 5.869847

42 H 7.727338 8.769182 8.388181 9.375840 6.410691

43 H 2.142937 3.300243 4.322587 5.605260 5.873788

44 H 2.142937 3.300243 4.322587 5.605260 5.873788

45 H 2.142037 2.761102 4.131587 5.249934 6.401561

26 27 28 29 30

26 C 0.000000

27 H 2.993977 0.000000

28 C 7.932142 9.466400 0.000000

29 H 5.288509 7.398695 2.985787 0.000000

30 C 7.923696 5.264585 11.216794 10.425058 0.000000

31 H 9.461280 7.373481 10.425058 10.458350 2.985787

32 C 11.206749 10.404426 7.923696 9.461280 7.932142

33 H 10.404426 10.432676 5.264585 7.373481 9.466400

34 H 1.092413 2.744295 9.024106 6.365600 7.964527

35 H 1.097548 3.748126 7.676855 4.951286 8.542651

36 H 1.097548 3.748126 7.676855 4.951286 8.542651

37 H 8.544732 9.954900 1.096965 3.737823 11.428696

38 H 8.544732 9.954900 1.096965 3.737823 11.428696

39 H 7.981793 9.818939 1.092154 2.739887 11.996222

40 H 7.661159 4.922452 11.428696 10.470311 1.096965

41 H 7.661159 4.922452 11.428696 10.470311 1.096965

42 H 9.015570 6.340562 11.996222 11.374335 1.092154

43 H 11.427763 10.458235 8.542651 9.958719 7.676855

44 H 11.427763 10.458235 8.542651 9.958719 7.676855

45 H 11.981745 11.351175 7.964527 9.804470 9.024106

31 32 33 34 35

31 H 0.000000

32 C 5.288509 0.000000

33 H 7.398695 2.993977 0.000000

34 H 9.804470 11.981745 11.351175 0.000000

35 H 9.958719 11.427763 10.458235 1.774874 0.000000

36 H 9.958719 11.427763 10.458235 1.774874 1.762181

37 H 10.470311 7.661159 4.922452 9.629616 8.215032

38 H 10.470311 7.661159 4.922452 9.629616 8.402026

39 H 11.374335 9.015570 6.340562 9.068745 7.648730

40 H 3.737823 8.544732 9.954900 7.625001 8.204811

41 H 3.737823 8.544732 9.954900 7.625001 8.392032

42 H 2.739887 7.981793 9.818939 9.050511 9.627753

43 H 4.951286 1.097548 3.748126 12.157818 11.614657

44 H 4.951286 1.097548 3.748126 12.157818 11.747576

45 H 6.365600 1.092413 2.744295 12.803121 12.157818

36 37 38 39 40

36 H 0.000000

37 H 8.402026 0.000000

38 H 8.215032 1.763315 0.000000

39 H 7.648730 1.776317 1.776317 0.000000

40 H 8.392032 11.606512 11.739693 12.163421 0.000000

41 H 8.204811 11.739693 11.606512 12.163421 1.763315

42 H 9.627753 12.163421 12.163421 12.821382 1.776317

43 H 11.747576 8.204811 8.392032 9.627753 8.215032

44 H 11.614657 8.392032 8.204811 9.627753 8.402026

45 H 12.157818 7.625001 7.625001 9.050511 9.629616

41 42 43 44 45

41 H 0.000000

42 H 1.776317 0.000000

43 H 8.402026 7.648730 0.000000

44 H 8.215032 7.648730 1.762181 0.000000

45 H 9.629616 9.068745 1.774874 1.774874 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=3 Diff= 8.61D-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 -2.945547 0.655244 0.000000

2 7 0 -1.981586 -0.330137 0.000000

3 6 0 -2.580425 -1.537618 0.000000

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5 6 0 -4.241675 0.018800 0.000000

6 7 0 -1.979086 -2.758973 0.000000

7 6 0 -0.660340 -2.933847 0.000000

8 7 0 0.302839 -1.978972 0.000000

9 6 0 1.540593 -2.577406 0.000000

10 6 0 1.340496 -4.053869 0.000000

11 6 0 0.000000 -4.258365 0.000000

12 7 0 -2.720334 1.991804 0.000000

13 6 0 -1.340496 4.053869 0.000000

14 6 0 0.000000 4.258365 0.000000

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16 7 0 -0.302839 1.978972 0.000000

17 6 0 -1.540593 2.577406 0.000000

18 7 0 1.979086 2.758973 0.000000

19 7 0 1.981586 0.330137 0.000000

20 6 0 2.580425 1.537618 0.000000

21 6 0 4.042735 1.342451 0.000000

22 6 0 4.241675 -0.018800 0.000000

23 6 0 2.945547 -0.655244 0.000000

24 7 0 2.720334 -1.991804 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -5.041167 -2.446312 0.000000

27 1 0 -5.187887 0.544068 0.000000

28 6 0 2.453878 -5.043074 0.000000

29 1 0 -0.527650 -5.202486 0.000000

30 6 0 -2.453878 5.043074 0.000000

31 1 0 0.527650 5.202486 0.000000

32 6 0 5.041167 2.446312 0.000000

33 1 0 5.187887 -0.544068 0.000000

34 1 0 -6.061970 -2.057304 0.000000

35 1 0 -4.917643 -3.088988 0.881091

36 1 0 -4.917643 -3.088988 -0.881091

37 1 0 3.092938 -4.910348 0.881658

38 1 0 3.092938 -4.910348 -0.881658

39 1 0 2.072452 -6.066457 0.000000

40 1 0 -3.092938 4.910348 0.881658

41 1 0 -3.092938 4.910348 -0.881658

42 1 0 -2.072452 6.066457 0.000000

43 1 0 4.917643 3.088988 0.881091

44 1 0 4.917643 3.088988 -0.881091

45 1 0 6.061970 2.057304 0.000000

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

Rotational constants (GHZ): 0.1826860 0.1820002 0.0913777

Leave Link 202 at Tue Sep 17 14:04:00 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 101 beta electrons

nuclear repulsion energy 2761.2964768779 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= -0.1141965899 Hartrees.

Nuclear repulsion after empirical dispersion term = 2761.1822802880 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 = 3602

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.44D-08

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 248

GePol: Fraction of low-weight points (<1% of avg) = 6.89%

GePol: Cavity surface area = 378.838 Ang\*\*2

GePol: Cavity volume = 378.313 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0107148636 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2761.1715654244 Hartrees.

Leave Link 301 at Tue Sep 17 14:04:00 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= 15333 LenP2D= 41264.

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 14:04:01 2019, MaxMem= 2415919104 cpu: 11.8

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:04:01 2019, MaxMem= 2415919104 cpu: 1.2

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.952541 0.000000 -0.000000 0.304411 Ang= 35.45 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 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0187 S= 1.0062

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= -1276.14492784915

Leave Link 401 at Tue Sep 17 14:04:03 2019, MaxMem= 2415919104 cpu: 38.9

(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= 38923212.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.33D-15 for 3601.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.61D-15 for 1828 158.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.88D-15 for 3601.

Iteration 1 A^-1\*A deviation from orthogonality is 6.54D-11 for 2497 2495.

E= -1275.84052284150

DIIS: error= 1.65D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.84052284150 IErMin= 1 ErrMin= 1.65D-03

ErrMax= 1.65D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.86D-03 BMatP= 3.86D-03

IDIUse=3 WtCom= 9.84D-01 WtEn= 1.65D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.302 Goal= None Shift= 0.000

Gap= 0.394 Goal= None Shift= 0.000

GapD= 0.302 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.

RMSDP=9.39D-05 MaxDP=2.32D-03 OVMax= 2.25D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 9.38D-05 CP: 1.00D+00

E= -1275.84180041418 Delta-E= -0.001277572689 Rises=F Damp=F

DIIS: error= 4.36D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84180041418 IErMin= 2 ErrMin= 4.36D-04

ErrMax= 4.36D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.67D-04 BMatP= 3.86D-03

IDIUse=3 WtCom= 9.96D-01 WtEn= 4.36D-03

Coeff-Com: 0.754D-01 0.925D+00

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

Coeff: 0.750D-01 0.925D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=2.83D-05 MaxDP=1.08D-03 DE=-1.28D-03 OVMax= 1.27D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.61D-05 CP: 1.00D+00 1.12D+00

E= -1275.84183400346 Delta-E= -0.000033589271 Rises=F Damp=F

DIIS: error= 3.80D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1275.84183400346 IErMin= 3 ErrMin= 3.80D-04

ErrMax= 3.80D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.40D-04 BMatP= 2.67D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.80D-03

Coeff-Com: -0.885D-02 0.487D+00 0.522D+00

Coeff-En: 0.000D+00 0.316D+00 0.684D+00

Coeff: -0.881D-02 0.486D+00 0.523D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.77D-05 MaxDP=8.92D-04 DE=-3.36D-05 OVMax= 8.95D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.67D-05 CP: 1.00D+00 1.15D+00 8.02D-01

E= -1275.84189486108 Delta-E= -0.000060857622 Rises=F Damp=F

DIIS: error= 2.34D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84189486108 IErMin= 4 ErrMin= 2.34D-04

ErrMax= 2.34D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.00D-05 BMatP= 2.40D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.34D-03

Coeff-Com: -0.977D-02 0.157D+00 0.313D+00 0.540D+00

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

Coeff: -0.975D-02 0.157D+00 0.312D+00 0.541D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=9.32D-06 MaxDP=3.84D-04 DE=-6.09D-05 OVMax= 5.88D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 5.62D-06 CP: 1.00D+00 1.18D+00 1.04D+00 1.16D+00

E= -1275.84191189713 Delta-E= -0.000017036056 Rises=F Damp=F

DIIS: error= 1.98D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84191189713 IErMin= 5 ErrMin= 1.98D-04

ErrMax= 1.98D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.22D-06 BMatP= 4.00D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.98D-03

Coeff-Com: -0.233D-02 0.807D-02 0.960D-01 0.227D+00 0.672D+00

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

Coeff: -0.233D-02 0.806D-02 0.959D-01 0.226D+00 0.672D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=9.52D-06 MaxDP=5.31D-04 DE=-1.70D-05 OVMax= 7.62D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.75D-06 CP: 1.00D+00 1.21D+00 1.22D+00 1.59D+00 1.25D+00

E= -1275.84192162687 Delta-E= -0.000009729737 Rises=F Damp=F

DIIS: error= 1.49D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84192162687 IErMin= 6 ErrMin= 1.49D-04

ErrMax= 1.49D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.07D-06 BMatP= 5.22D-06

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.49D-03

Coeff-Com: 0.389D-02-0.781D-01-0.906D-01-0.214D+00 0.497D+00 0.883D+00

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

Coeff: 0.388D-02-0.780D-01-0.904D-01-0.214D+00 0.496D+00 0.883D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.37D-05 MaxDP=6.78D-04 DE=-9.73D-06 OVMax= 1.08D-02

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.77D-06 CP: 1.00D+00 1.25D+00 1.51D+00 2.15D+00 2.08D+00

CP: 1.65D+00

E= -1275.84193372927 Delta-E= -0.000012102402 Rises=F Damp=F

DIIS: error= 1.16D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84193372927 IErMin= 7 ErrMin= 1.16D-04

ErrMax= 1.16D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.98D-06 BMatP= 5.07D-06

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.16D-03

Coeff-Com: 0.500D-02-0.650D-01-0.125D+00-0.347D+00 0.571D-01 0.317D+00

Coeff-Com: 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: 0.100D+01

Coeff: 0.499D-02-0.649D-01-0.125D+00-0.346D+00 0.570D-01 0.316D+00

Coeff: 0.116D+01

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.82D-05 MaxDP=9.23D-04 DE=-1.21D-05 OVMax= 1.46D-02

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.65D-06 CP: 1.00D+00 1.30D+00 1.87D+00 2.92D+00 3.00D+00

CP: 2.89D+00 1.96D+00

E= -1275.84194416677 Delta-E= -0.000010437493 Rises=F Damp=F

DIIS: error= 6.77D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84194416677 IErMin= 8 ErrMin= 6.77D-05

ErrMax= 6.77D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.30D-06 BMatP= 1.98D-06

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

Coeff-Com: -0.625D-03 0.286D-01 0.212D-01 0.345D-02-0.190D+00-0.782D+00

Coeff-Com: 0.806D+00 0.111D+01

Coeff: -0.625D-03 0.286D-01 0.212D-01 0.345D-02-0.190D+00-0.782D+00

Coeff: 0.806D+00 0.111D+01

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.57D-05 MaxDP=7.78D-04 DE=-1.04D-05 OVMax= 1.24D-02

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.10D-05 CP: 1.00D+00 1.35D+00 2.18D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.75D+00

E= -1275.84194891235 Delta-E= -0.000004745582 Rises=F Damp=F

DIIS: error= 2.07D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84194891235 IErMin= 9 ErrMin= 2.07D-05

ErrMax= 2.07D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.27D-07 BMatP= 1.30D-06

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

Coeff-Com: -0.205D-02 0.384D-01 0.582D-01 0.130D+00-0.950D-01-0.588D+00

Coeff-Com: 0.111D+00 0.614D+00 0.734D+00

Coeff: -0.205D-02 0.384D-01 0.582D-01 0.130D+00-0.950D-01-0.588D+00

Coeff: 0.111D+00 0.614D+00 0.734D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.47D-06 MaxDP=2.15D-04 DE=-4.75D-06 OVMax= 3.46D-03

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.29D-06 CP: 1.00D+00 1.36D+00 2.26D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.31D+00

E= -1275.84194954250 Delta-E= -0.000000630156 Rises=F Damp=F

DIIS: error= 1.15D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84194954250 IErMin=10 ErrMin= 1.15D-05

ErrMax= 1.15D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.26D-07 BMatP= 3.27D-07

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

Coeff-Com: -0.858D-03 0.831D-02 0.245D-01 0.803D-01 0.423D-01 0.101D-01

Coeff-Com: -0.302D+00-0.163D+00 0.466D+00 0.835D+00

Coeff: -0.858D-03 0.831D-02 0.245D-01 0.803D-01 0.423D-01 0.101D-01

Coeff: -0.302D+00-0.163D+00 0.466D+00 0.835D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.97D-06 MaxDP=8.62D-05 DE=-6.30D-07 OVMax= 1.42D-03

Cycle 11 Pass 1 IDiag 1:

RMSU= 5.86D-07 CP: 1.00D+00 1.37D+00 2.29D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.44D+00 1.57D+00

E= -1275.84194973869 Delta-E= -0.000000196187 Rises=F Damp=F

DIIS: error= 5.70D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84194973869 IErMin=11 ErrMin= 5.70D-06

ErrMax= 5.70D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.88D-08 BMatP= 1.26D-07

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

Coeff-Com: 0.210D-03-0.682D-02-0.678D-02-0.829D-02 0.324D-01 0.132D+00

Coeff-Com: -0.102D+00-0.199D+00-0.410D-01 0.195D+00 0.100D+01

Coeff: 0.210D-03-0.682D-02-0.678D-02-0.829D-02 0.324D-01 0.132D+00

Coeff: -0.102D+00-0.199D+00-0.410D-01 0.195D+00 0.100D+01

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.17D-06 MaxDP=5.15D-05 DE=-1.96D-07 OVMax= 8.37D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.91D-07 CP: 1.00D+00 1.37D+00 2.31D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.52D+00 1.93D+00

CP: 1.42D+00

E= -1275.84194978783 Delta-E= -0.000000049135 Rises=F Damp=F

DIIS: error= 3.01D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84194978783 IErMin=12 ErrMin= 3.01D-06

ErrMax= 3.01D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.08D-08 BMatP= 1.88D-08

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

Coeff-Com: 0.343D-03-0.620D-02-0.995D-02-0.249D-01 0.117D-01 0.786D-01

Coeff-Com: 0.144D-01-0.866D-01-0.140D+00-0.899D-01 0.624D+00 0.629D+00

Coeff: 0.343D-03-0.620D-02-0.995D-02-0.249D-01 0.117D-01 0.786D-01

Coeff: 0.144D-01-0.866D-01-0.140D+00-0.899D-01 0.624D+00 0.629D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.75D-07 MaxDP=1.38D-05 DE=-4.91D-08 OVMax= 1.50D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.05D-07 CP: 1.00D+00 1.37D+00 2.32D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.53D+00 2.03D+00

CP: 1.62D+00 1.17D+00

E= -1275.84194979671 Delta-E= -0.000000008888 Rises=F Damp=F

DIIS: error= 1.20D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84194979671 IErMin=13 ErrMin= 1.20D-06

ErrMax= 1.20D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.71D-09 BMatP= 1.08D-08

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

Coeff-Com: 0.514D-04 0.165D-03-0.111D-02-0.629D-02-0.696D-02-0.191D-01

Coeff-Com: 0.397D-01 0.350D-01-0.366D-01-0.978D-01-0.107D+00 0.230D+00

Coeff-Com: 0.969D+00

Coeff: 0.514D-04 0.165D-03-0.111D-02-0.629D-02-0.696D-02-0.191D-01

Coeff: 0.397D-01 0.350D-01-0.366D-01-0.978D-01-0.107D+00 0.230D+00

Coeff: 0.969D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.81D-07 MaxDP=1.11D-05 DE=-8.89D-09 OVMax= 1.96D-04

Cycle 14 Pass 1 IDiag 1:

RMSU= 4.97D-08 CP: 1.00D+00 1.37D+00 2.32D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.55D+00 2.11D+00

CP: 1.73D+00 1.48D+00 1.19D+00

E= -1275.84194979948 Delta-E= -0.000000002762 Rises=F Damp=F

DIIS: error= 7.40D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84194979948 IErMin=14 ErrMin= 7.40D-07

ErrMax= 7.40D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.75D-10 BMatP= 1.71D-09

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

Coeff-Com: -0.486D-04 0.158D-02 0.165D-02 0.195D-02-0.750D-02-0.318D-01

Coeff-Com: 0.219D-01 0.433D-01 0.854D-02-0.395D-01-0.214D+00 0.104D-01

Coeff-Com: 0.643D+00 0.561D+00

Coeff: -0.486D-04 0.158D-02 0.165D-02 0.195D-02-0.750D-02-0.318D-01

Coeff: 0.219D-01 0.433D-01 0.854D-02-0.395D-01-0.214D+00 0.104D-01

Coeff: 0.643D+00 0.561D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.12D-07 MaxDP=4.94D-06 DE=-2.76D-09 OVMax= 8.15D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 2.37D-08 CP: 1.00D+00 1.37D+00 2.32D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.56D+00 2.13D+00

CP: 1.77D+00 1.55D+00 1.34D+00 1.09D+00

E= -1275.84194979988 Delta-E= -0.000000000403 Rises=F Damp=F

DIIS: error= 2.46D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.84194979988 IErMin=15 ErrMin= 2.46D-07

ErrMax= 2.46D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.96D-11 BMatP= 8.75D-10

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

Coeff-Com: -0.210D-04 0.373D-03 0.634D-03 0.176D-02-0.865D-03-0.531D-02

Coeff-Com: -0.794D-03 0.699D-02 0.724D-02 0.881D-02-0.417D-01-0.424D-01

Coeff-Com: 0.242D-02 0.141D+00 0.922D+00

Coeff: -0.210D-04 0.373D-03 0.634D-03 0.176D-02-0.865D-03-0.531D-02

Coeff: -0.794D-03 0.699D-02 0.724D-02 0.881D-02-0.417D-01-0.424D-01

Coeff: 0.242D-02 0.141D+00 0.922D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.24D-08 MaxDP=1.06D-06 DE=-4.03D-10 OVMax= 1.16D-05

Cycle 16 Pass 1 IDiag 1:

RMSU= 1.00D-08 CP: 1.00D+00 1.37D+00 2.32D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.56D+00 2.14D+00

CP: 1.77D+00 1.60D+00 1.41D+00 1.25D+00 1.05D+00

E= -1275.84194979996 Delta-E= -0.000000000078 Rises=F Damp=F

DIIS: error= 1.91D-07 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1275.84194979996 IErMin=16 ErrMin= 1.91D-07

ErrMax= 1.91D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.25D-11 BMatP= 5.96D-11

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

Coeff-Com: -0.314D-05-0.779D-04 0.563D-04 0.715D-03 0.788D-03 0.315D-02

Coeff-Com: -0.506D-02-0.403D-02 0.277D-02 0.135D-01 0.160D-01-0.305D-01

Coeff-Com: -0.125D+00-0.321D-01 0.552D+00 0.607D+00

Coeff: -0.314D-05-0.779D-04 0.563D-04 0.715D-03 0.788D-03 0.315D-02

Coeff: -0.506D-02-0.403D-02 0.277D-02 0.135D-01 0.160D-01-0.305D-01

Coeff: -0.125D+00-0.321D-01 0.552D+00 0.607D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=8.57D-09 MaxDP=7.03D-07 DE=-7.82D-11 OVMax= 3.29D-06

Error on total polarization charges = 0.06486

SCF Done: E(UB3LYP) = -1275.84194980 A.U. after 16 cycles

NFock= 16 Conv=0.86D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0224 S= 1.0075

<L.S>= 0.000000000000E+00

KE= 1.320762134438D+03 PE=-8.574316226417D+03 EE= 3.216540576755D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.72

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0224, after 2.0003

Leave Link 502 at Tue Sep 17 14:05:34 2019, MaxMem= 2415919104 cpu: 1602.9

(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= 15333 LenP2D= 41264.

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 14:05:39 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 14:05:39 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 14:05:51 2019, MaxMem= 2415919104 cpu: 215.2

(Enter /home/blab/g09/l716.exe)

Dipole =-1.58095759D-13 1.86961557D-13-8.88178420D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.006704852 -0.001796742 0.000000000

2 7 -0.003184815 0.000439345 -0.000000000

3 6 -0.001400522 -0.000232082 -0.000000000

4 6 -0.001038450 0.002527105 -0.000000000

5 6 0.000018889 -0.001157179 0.000000000

6 7 0.004818673 0.000640769 0.000000000

7 6 -0.004130474 -0.004140929 -0.000000000

8 7 0.001021560 0.003055985 0.000000000

9 6 -0.006414559 0.003927382 -0.000000000

10 6 0.003002276 -0.005798961 -0.000000000

11 6 0.002931771 0.004555350 0.000000000

12 7 -0.007360754 0.003950078 0.000000000

13 6 -0.003002276 0.005798961 0.000000000

14 6 -0.002931771 -0.004555350 0.000000000

15 6 0.004130474 0.004140929 0.000000000

16 7 -0.001021560 -0.003055985 -0.000000000

17 6 0.006414559 -0.003927382 0.000000000

18 7 -0.004818673 -0.000640769 0.000000000

19 7 0.003184815 -0.000439345 -0.000000000

20 6 0.001400522 0.000232082 -0.000000000

21 6 0.001038450 -0.002527105 0.000000000

22 6 -0.000018889 0.001157179 0.000000000

23 6 -0.006704852 0.001796742 -0.000000000

24 7 0.007360754 -0.003950078 0.000000000

25 30 0.000000000 -0.000000000 0.000000000

26 6 0.000364650 -0.000094300 -0.000000000

27 1 0.000634953 0.000314394 0.000000000

28 6 -0.000705089 -0.000153611 0.000000000

29 1 -0.000246836 0.000301322 -0.000000000

30 6 0.000705089 0.000153611 -0.000000000

31 1 0.000246836 -0.000301322 -0.000000000

32 6 -0.000364650 0.000094300 -0.000000000

33 1 -0.000634953 -0.000314394 0.000000000

34 1 0.000616843 0.000320765 0.000000000

35 1 -0.000477752 0.000050014 -0.001555643

36 1 -0.000477752 0.000050014 0.001555643

37 1 -0.000280958 -0.000441885 -0.001626370

38 1 -0.000280958 -0.000441885 0.001626370

39 1 -0.000390065 0.000690563 0.000000000

40 1 0.000280958 0.000441885 -0.001626370

41 1 0.000280958 0.000441885 0.001626370

42 1 0.000390065 -0.000690563 -0.000000000

43 1 0.000477752 -0.000050014 -0.001555643

44 1 0.000477752 -0.000050014 0.001555643

45 1 -0.000616843 -0.000320765 -0.000000000

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

Cartesian Forces: Max 0.007360754 RMS 0.002275380

Leave Link 716 at Tue Sep 17 14:05:51 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 0.004756350 RMS 0.000958115

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= -3.45D-04 DEPred=-8.77D-04 R= 3.93D-01

Trust test= 3.93D-01 RLast= 1.06D-01 DXMaxT set to 2.52D-01

ITU= 0 1 -1 1 1 1 1 0 0

Eigenvalues --- 0.00214 0.00878 0.00878 0.00878 0.00878

Eigenvalues --- 0.01336 0.01338 0.01342 0.01343 0.01604

Eigenvalues --- 0.01623 0.01633 0.01639 0.01774 0.01791

Eigenvalues --- 0.01810 0.01818 0.01888 0.01905 0.01938

Eigenvalues --- 0.01947 0.01997 0.01999 0.02043 0.02048

Eigenvalues --- 0.02070 0.02087 0.02102 0.02110 0.02114

Eigenvalues --- 0.02205 0.02313 0.02319 0.02352 0.02374

Eigenvalues --- 0.04114 0.07070 0.07224 0.07224 0.07251

Eigenvalues --- 0.07251 0.07335 0.07377 0.07438 0.13404

Eigenvalues --- 0.14487 0.14510 0.15605 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16004 0.16011

Eigenvalues --- 0.16034 0.16156 0.16328 0.18280 0.20812

Eigenvalues --- 0.22066 0.22097 0.23848 0.23850 0.23858

Eigenvalues --- 0.24481 0.24997 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25006 0.25025

Eigenvalues --- 0.26089 0.27875 0.30536 0.33192 0.33197

Eigenvalues --- 0.33248 0.33282 0.33282 0.33345 0.33549

Eigenvalues --- 0.33714 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33724 0.34383 0.34436 0.34437

Eigenvalues --- 0.34437 0.34614 0.35253 0.35559 0.35561

Eigenvalues --- 0.35607 0.35682 0.35682 0.35789 0.36559

Eigenvalues --- 0.38515 0.40591 0.41662 0.41797 0.44474

Eigenvalues --- 0.47876 0.48704 0.48944 0.49002 0.51157

Eigenvalues --- 0.51354 0.51365 0.52660 0.53982 0.54028

Eigenvalues --- 0.54622 0.56313 0.56352 0.57111

Cosine: 0.395 < 0.710

Cut down GDIIS temporarily because of the cosine check. E 7

DIIS coeff's: 3.34816 -3.94004 1.59189

Cosine: 0.905 > 0.840

Length: 0.854

GDIIS step was calculated using 3 of the last 9 vectors.

Maximum step size ( 0.252) exceeded in Quadratic search.

-- Step size scaled by 0.090

Iteration 1 RMS(Cart)= 0.02848845 RMS(Int)= 0.00021963

Iteration 2 RMS(Cart)= 0.00044732 RMS(Int)= 0.00004592

Iteration 3 RMS(Cart)= 0.00000006 RMS(Int)= 0.00004592

ITry= 1 IFail=0 DXMaxC= 1.12D-01 DCOld= 1.00D+10 DXMaxT= 2.52D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 4.43D-10 for atom 27.

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

(Linear) (Quad) (Total)

R1 2.60494 -0.00150 0.00133 -0.03944 -0.03828 2.56666

R2 2.72868 -0.00037 -0.00046 0.00704 0.00655 2.73523

R3 2.56134 0.00476 -0.00018 0.05497 0.05483 2.61617

R4 2.54701 0.00037 -0.00121 0.03498 0.03370 2.58071

R5 3.79627 -0.00090 -0.00091 0.04742 0.04633 3.84260

R6 2.78787 -0.00134 0.00088 -0.04817 -0.04720 2.74067

R7 2.57261 0.00257 0.00057 0.00061 0.00126 2.57387

R8 2.59972 -0.00154 -0.00084 0.00064 -0.00008 2.59964

R9 2.81269 -0.00030 -0.00054 0.01798 0.01744 2.83014

R10 2.04512 -0.00071 -0.00022 -0.00914 -0.00936 2.03576

R11 2.51389 -0.00274 0.00005 -0.00497 -0.00482 2.50907

R12 2.56300 0.00177 -0.00081 0.03520 0.03443 2.59743

R13 2.79679 0.00146 0.00087 -0.01275 -0.01183 2.78496

R14 2.59805 -0.00117 0.00101 -0.03169 -0.03068 2.56737

R15 3.78325 -0.00090 -0.00110 0.06469 0.06354 3.84679

R16 2.81562 0.00314 0.00043 0.02209 0.02250 2.83811

R17 2.48893 -0.00200 -0.00095 0.02399 0.02312 2.51205

R18 2.56248 -0.00439 -0.00123 -0.00660 -0.00779 2.55469

R19 2.81445 -0.00168 -0.00052 -0.02390 -0.02442 2.79003

R20 2.04386 -0.00038 -0.00021 0.00395 0.00374 2.04760

R21 2.48893 -0.00200 -0.00095 0.02399 0.02312 2.51205

R22 2.56248 -0.00439 -0.00123 -0.00660 -0.00779 2.55469

R23 2.81562 0.00314 0.00043 0.02209 0.02250 2.83811

R24 2.81445 -0.00168 -0.00052 -0.02390 -0.02442 2.79003

R25 2.79679 0.00146 0.00087 -0.01275 -0.01183 2.78496

R26 2.04386 -0.00038 -0.00021 0.00395 0.00374 2.04760

R27 2.56300 0.00177 -0.00081 0.03520 0.03443 2.59743

R28 2.51389 -0.00274 0.00005 -0.00497 -0.00482 2.50907

R29 2.59805 -0.00117 0.00101 -0.03169 -0.03068 2.56737

R30 3.78325 -0.00090 -0.00110 0.06469 0.06354 3.84679

R31 2.57261 0.00257 0.00057 0.00061 0.00126 2.57387

R32 2.54701 0.00037 -0.00121 0.03498 0.03370 2.58071

R33 2.60494 -0.00150 0.00133 -0.03944 -0.03828 2.56666

R34 3.79627 -0.00090 -0.00091 0.04742 0.04633 3.84260

R35 2.78787 -0.00134 0.00088 -0.04817 -0.04720 2.74067

R36 2.59972 -0.00154 -0.00084 0.00064 -0.00008 2.59964

R37 2.81269 -0.00030 -0.00054 0.01798 0.01744 2.83014

R38 2.72868 -0.00037 -0.00046 0.00704 0.00655 2.73523

R39 2.04512 -0.00071 -0.00022 -0.00914 -0.00936 2.03576

R40 2.56134 0.00476 -0.00018 0.05497 0.05483 2.61617

R41 2.06436 -0.00068 -0.00028 -0.00532 -0.00560 2.05876

R42 2.07407 -0.00153 -0.00064 -0.01202 -0.01266 2.06140

R43 2.07407 -0.00153 -0.00064 -0.01202 -0.01266 2.06140

R44 2.07296 -0.00161 -0.00068 -0.01486 -0.01554 2.05743

R45 2.07296 -0.00161 -0.00068 -0.01486 -0.01554 2.05743

R46 2.06387 -0.00078 -0.00030 -0.00764 -0.00794 2.05593

R47 2.07296 -0.00161 -0.00068 -0.01486 -0.01554 2.05743

R48 2.07296 -0.00161 -0.00068 -0.01486 -0.01554 2.05743

R49 2.06387 -0.00078 -0.00030 -0.00764 -0.00794 2.05593

R50 2.07407 -0.00153 -0.00064 -0.01202 -0.01266 2.06140

R51 2.07407 -0.00153 -0.00064 -0.01202 -0.01266 2.06140

R52 2.06436 -0.00068 -0.00028 -0.00532 -0.00560 2.05876

A1 1.88876 0.00007 -0.00017 -0.00788 -0.00819 1.88057

A2 2.20025 0.00060 0.00011 0.02141 0.02148 2.22172

A3 2.19418 -0.00067 0.00006 -0.01353 -0.01329 2.18089

A4 1.90679 0.00026 0.00012 0.01810 0.01824 1.92503

A5 2.18012 0.00077 0.00004 0.00600 0.00600 2.18612

A6 2.19628 -0.00103 -0.00016 -0.02410 -0.02425 2.17203

A7 1.89851 -0.00089 -0.00032 -0.02297 -0.02331 1.87520

A8 2.22369 0.00095 0.00118 -0.00614 -0.00500 2.21868

A9 2.16099 -0.00007 -0.00085 0.02911 0.02831 2.18930

A10 1.84859 0.00098 0.00039 0.02215 0.02266 1.87126

A11 2.17341 -0.00066 -0.00084 0.00393 0.00303 2.17644

A12 2.26119 -0.00032 0.00045 -0.02609 -0.02569 2.23549

A13 1.88213 -0.00042 -0.00002 -0.00940 -0.00941 1.87272

A14 2.17837 0.00026 -0.00004 0.01257 0.01252 2.19089

A15 2.22268 0.00016 0.00007 -0.00317 -0.00311 2.21958

A16 2.16015 -0.00104 -0.00188 0.04416 0.04238 2.20253

A17 2.22869 0.00084 0.00079 -0.00838 -0.00757 2.22112

A18 2.16512 -0.00013 -0.00061 0.02366 0.02302 2.18815

A19 1.88938 -0.00071 -0.00018 -0.01528 -0.01545 1.87392

A20 1.91018 -0.00016 0.00013 0.01144 0.01161 1.92178

A21 2.20001 -0.00050 0.00020 -0.02652 -0.02637 2.17365

A22 2.17299 0.00066 -0.00033 0.01508 0.01476 2.18775

A23 1.88644 -0.00035 -0.00039 -0.00505 -0.00554 1.88090

A24 2.23050 0.00199 0.00084 0.00826 0.00915 2.23965

A25 2.16625 -0.00164 -0.00045 -0.00321 -0.00361 2.16264

A26 1.85688 0.00032 0.00015 -0.00184 -0.00169 1.85519

A27 2.16250 -0.00069 -0.00054 0.01909 0.01855 2.18105

A28 2.26380 0.00037 0.00039 -0.01725 -0.01686 2.24694

A29 1.88190 0.00090 0.00029 0.01073 0.01108 1.89298

A30 2.16947 -0.00051 -0.00035 0.00780 0.00742 2.17689

A31 2.23182 -0.00039 0.00006 -0.01853 -0.01851 2.21331

A32 2.19848 -0.00324 -0.00078 -0.02977 -0.03058 2.16790

A33 1.85688 0.00032 0.00015 -0.00184 -0.00169 1.85519

A34 2.26380 0.00037 0.00039 -0.01725 -0.01686 2.24694

A35 2.16250 -0.00069 -0.00054 0.01909 0.01855 2.18105

A36 1.88190 0.00090 0.00029 0.01073 0.01108 1.89298

A37 2.23182 -0.00039 0.00006 -0.01853 -0.01851 2.21331

A38 2.16947 -0.00051 -0.00035 0.00780 0.00742 2.17689

A39 1.88938 -0.00071 -0.00018 -0.01528 -0.01545 1.87392

A40 2.16512 -0.00013 -0.00061 0.02366 0.02302 2.18815

A41 2.22869 0.00084 0.00079 -0.00838 -0.00757 2.22112

A42 1.91018 -0.00016 0.00013 0.01144 0.01161 1.92178

A43 2.20001 -0.00050 0.00020 -0.02652 -0.02637 2.17365

A44 2.17299 0.00066 -0.00033 0.01508 0.01476 2.18775

A45 2.16625 -0.00164 -0.00045 -0.00321 -0.00361 2.16264

A46 2.23050 0.00199 0.00084 0.00826 0.00915 2.23965

A47 1.88644 -0.00035 -0.00039 -0.00505 -0.00554 1.88090

A48 2.16015 -0.00104 -0.00188 0.04416 0.04238 2.20253

A49 1.90679 0.00026 0.00012 0.01810 0.01824 1.92503

A50 2.19628 -0.00103 -0.00016 -0.02410 -0.02425 2.17203

A51 2.18012 0.00077 0.00004 0.00600 0.00600 2.18612

A52 2.22369 0.00095 0.00118 -0.00614 -0.00500 2.21868

A53 2.16099 -0.00007 -0.00085 0.02911 0.02831 2.18930

A54 1.89851 -0.00089 -0.00032 -0.02297 -0.02331 1.87520

A55 1.84859 0.00098 0.00039 0.02215 0.02266 1.87126

A56 2.17341 -0.00066 -0.00084 0.00393 0.00303 2.17644

A57 2.26119 -0.00032 0.00045 -0.02609 -0.02569 2.23549

A58 1.88213 -0.00042 -0.00002 -0.00940 -0.00941 1.87272

A59 2.22268 0.00016 0.00007 -0.00317 -0.00311 2.21958

A60 2.17837 0.00026 -0.00004 0.01257 0.01252 2.19089

A61 1.88876 0.00007 -0.00017 -0.00788 -0.00819 1.88057

A62 2.20025 0.00060 0.00011 0.02141 0.02148 2.22172

A63 2.19418 -0.00067 0.00006 -0.01353 -0.01329 2.18089

A64 2.19848 -0.00324 -0.00078 -0.02977 -0.03058 2.16790

A65 1.55756 0.00078 -0.00013 0.02097 0.02080 1.57836

A66 1.58403 -0.00078 0.00013 -0.02097 -0.02080 1.56323

A67 1.58403 -0.00078 0.00013 -0.02097 -0.02080 1.56323

A68 1.55756 0.00078 -0.00013 0.02097 0.02080 1.57836

A69 1.94200 0.00013 0.00057 -0.01552 -0.01488 1.92711

A70 1.93775 0.00038 0.00010 0.01567 0.01573 1.95348

A71 1.93775 0.00038 0.00010 0.01567 0.01573 1.95348

A72 1.88987 -0.00013 0.00006 -0.00225 -0.00213 1.88774

A73 1.88987 -0.00013 0.00006 -0.00225 -0.00213 1.88774

A74 1.86389 -0.00068 -0.00096 -0.01191 -0.01301 1.85088

A75 1.93387 0.00010 0.00005 0.00161 0.00166 1.93552

A76 1.93387 0.00010 0.00005 0.00161 0.00166 1.93552

A77 1.94044 0.00029 0.00057 -0.00962 -0.00905 1.93139

A78 1.86706 -0.00057 -0.00087 -0.00999 -0.01086 1.85620

A79 1.89319 0.00002 0.00008 0.00836 0.00844 1.90163

A80 1.89319 0.00002 0.00008 0.00836 0.00844 1.90163

A81 1.93387 0.00010 0.00005 0.00161 0.00166 1.93552

A82 1.93387 0.00010 0.00005 0.00161 0.00166 1.93552

A83 1.94044 0.00029 0.00057 -0.00962 -0.00905 1.93139

A84 1.86706 -0.00057 -0.00087 -0.00999 -0.01086 1.85620

A85 1.89319 0.00002 0.00008 0.00836 0.00844 1.90163

A86 1.89319 0.00002 0.00008 0.00836 0.00844 1.90163

A87 1.93775 0.00038 0.00010 0.01567 0.01573 1.95348

A88 1.93775 0.00038 0.00010 0.01567 0.01573 1.95348

A89 1.94200 0.00013 0.00057 -0.01552 -0.01488 1.92711

A90 1.86389 -0.00068 -0.00096 -0.01191 -0.01301 1.85088

A91 1.88987 -0.00013 0.00006 -0.00225 -0.00213 1.88774

A92 1.88987 -0.00013 0.00006 -0.00225 -0.00213 1.88774

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 1.03535 -0.00018 -0.00054 0.00270 0.00224 1.03758

D31 -1.03535 0.00018 0.00054 -0.00270 -0.00224 -1.03758

D32 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.10625 -0.00018 -0.00054 0.00270 0.00224 -2.10401

D34 2.10625 0.00018 0.00054 -0.00270 -0.00224 2.10401

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 1.03482 -0.00029 -0.00051 -0.00519 -0.00571 1.02912

D64 -1.03482 0.00029 0.00051 0.00519 0.00571 -1.02912

D65 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D66 -2.10677 -0.00029 -0.00051 -0.00519 -0.00571 -2.11247

D67 2.10677 0.00029 0.00051 0.00519 0.00571 2.11247

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 -2.10677 -0.00029 -0.00051 -0.00519 -0.00571 -2.11247

D80 2.10677 0.00029 0.00051 0.00519 0.00571 2.11247

D81 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D82 1.03482 -0.00029 -0.00051 -0.00519 -0.00571 1.02912

D83 -1.03482 0.00029 0.00051 0.00519 0.00571 -1.02912

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 1.03535 -0.00018 -0.00054 0.00270 0.00224 1.03758

D126 -1.03535 0.00018 0.00054 -0.00270 -0.00224 -1.03758

D127 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D128 -2.10625 -0.00018 -0.00054 0.00270 0.00224 -2.10401

D129 2.10625 0.00018 0.00054 -0.00270 -0.00224 2.10401

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 0.004756 0.000450 NO

RMS Force 0.000958 0.000300 NO

Maximum Displacement 0.112139 0.001800 NO

RMS Displacement 0.028296 0.001200 NO

Predicted change in Energy=-1.626175D-03

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:05:51 2019, MaxMem= 2415919104 cpu: 1.5

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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1 6 0 -2.071456 -2.208391 0.000000

2 7 0 -0.751186 -1.889577 0.000000

3 6 0 0.009945 -3.023462 0.000000

4 6 0 -0.896585 -4.155528 0.000000

5 6 0 -2.176779 -3.651978 0.000000

6 7 0 1.369786 -3.100664 0.000000

7 6 0 2.213347 -2.075335 0.000000

8 7 0 1.897271 -0.737671 0.000000

9 6 0 3.031431 0.010302 0.000000

10 6 0 4.201432 -0.931345 0.000000

11 6 0 3.683360 -2.180021 0.000000

12 7 0 -3.145386 -1.334730 0.000000

13 6 0 -4.201432 0.931345 0.000000

14 6 0 -3.683360 2.180021 0.000000

15 6 0 -2.213347 2.075335 0.000000

16 7 0 -1.897271 0.737671 0.000000

17 6 0 -3.031431 -0.010302 0.000000

18 7 0 -1.369786 3.100664 0.000000

19 7 0 0.751186 1.889577 0.000000

20 6 0 -0.009945 3.023462 0.000000

21 6 0 0.896585 4.155528 0.000000

22 6 0 2.176779 3.651978 0.000000

23 6 0 2.071456 2.208391 0.000000

24 7 0 3.145386 1.334730 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.468410 -5.590660 0.000000

27 1 0 -3.096721 -4.212544 0.000000

28 6 0 5.619180 -0.519267 0.000000

29 1 0 4.235793 -3.112157 0.000000

30 6 0 -5.619180 0.519267 0.000000

31 1 0 -4.235793 3.112157 0.000000

32 6 0 0.468410 5.590660 0.000000

33 1 0 3.096721 4.212544 0.000000

34 1 0 -1.338162 -6.246731 0.000000

35 1 0 0.140950 -5.833933 0.871463

36 1 0 0.140950 -5.833933 -0.871463

37 1 0 5.845732 0.092688 0.871519

38 1 0 5.845732 0.092688 -0.871519

39 1 0 6.271914 -1.389657 0.000000

40 1 0 -5.845732 -0.092688 0.871519

41 1 0 -5.845732 -0.092688 -0.871519

42 1 0 -6.271914 1.389657 0.000000

43 1 0 -0.140950 5.833933 0.871463

44 1 0 -0.140950 5.833933 -0.871463

45 1 0 1.338162 6.246731 0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.358218 0.000000

3 C 2.235300 1.365655 0.000000

4 C 2.274130 2.270611 1.450301 0.000000

5 C 1.447424 2.266798 2.275257 1.375668 0.000000

6 N 3.555038 2.442386 1.362031 2.499835 3.589161

7 C 4.286868 2.970347 2.398734 3.741508 4.664656

8 N 4.232471 2.888116 2.964261 4.414452 5.009099

9 C 5.564356 4.232934 4.281717 5.725684 6.366926

10 C 6.401559 5.044465 4.684604 6.032009 6.934221

11 C 5.754886 4.444047 3.769001 4.987838 6.042176

12 N 1.384417 2.457652 3.578817 3.607494 2.511541

13 C 3.794040 4.456658 5.777212 6.066159 5.010595

14 C 4.675082 5.015902 6.380966 6.921365 6.023453

15 C 4.286075 4.225925 5.562441 6.368479 5.727429

16 N 2.951207 2.866347 4.217059 4.994474 4.398538

17 C 2.398573 2.954860 4.281250 4.662668 3.740619

18 N 5.355222 5.028437 6.277625 7.271606 6.800691

19 N 4.976007 4.066833 4.968641 6.265657 6.267520

20 C 5.623354 4.968641 6.046956 7.233535 7.018309

21 C 7.022018 6.265657 7.233535 8.502301 8.390633

22 C 7.238192 6.267520 7.018309 8.390633 8.503013

23 C 6.055715 4.976007 5.623354 7.022018 7.238192

24 N 6.306278 5.057611 5.368876 6.817658 7.293332

25 Zn 3.027857 2.033417 3.023478 4.251151 4.251507

26 C 3.742926 3.711869 2.611385 1.497643 2.583992

27 H 2.251177 3.301168 3.326453 2.200875 1.077278

28 C 7.873946 6.516081 6.142842 7.461742 8.401837

29 H 6.371670 5.134653 4.226779 5.237359 6.435254

30 C 4.475094 5.431381 6.651164 6.645045 5.408272

31 H 5.743918 6.095887 7.461374 7.998098 7.070577

32 C 8.202202 7.579008 8.626313 9.841311 9.613708

33 H 8.242479 7.214033 7.866890 9.272062 9.468923

34 H 4.104377 4.396513 3.493832 2.137316 2.726908

35 H 4.335752 4.136822 2.945397 2.157074 3.300341

36 H 4.335752 4.136822 2.945397 2.157074 3.300341

37 H 8.290740 6.943216 6.672806 8.016591 8.896221

38 H 8.290740 6.943216 6.672806 8.016591 8.896221

39 H 8.383445 7.040870 6.471598 7.683581 8.746343

40 H 4.413718 5.471998 6.605901 6.462219 5.185490

41 H 4.413718 5.471998 6.605901 6.462219 5.185490

42 H 5.530805 6.421201 7.677068 7.722904 6.495245

43 H 8.316567 7.796438 8.901441 10.055833 9.740973

44 H 8.316567 7.796438 8.901441 10.055833 9.740973

45 H 9.116720 8.400291 9.364862 10.639601 10.504249

6 7 8 9 10

6 N 0.000000

7 C 1.327741 0.000000

8 N 2.421152 1.374500 0.000000

9 C 3.526921 2.240344 1.358595 0.000000

10 C 3.567094 2.293729 2.312285 1.501865 0.000000

11 C 2.490022 1.473736 2.295754 2.285284 1.351884

12 N 4.848227 5.409669 5.077881 6.321565 7.357884

13 C 6.877177 7.084455 6.322957 7.291270 8.606841

14 C 7.308893 7.271809 6.297330 7.056635 8.476469

15 C 6.295221 6.068252 4.980982 5.636671 7.084455

16 N 5.040484 4.980982 4.071263 4.982085 6.322957

17 C 5.377830 5.636671 4.982085 6.062898 7.291270

18 N 6.779508 6.295221 5.040484 5.377830 6.877177

19 N 5.028437 4.225925 2.866347 2.954860 4.456658

20 C 6.277625 5.562441 4.217059 4.281250 5.777212

21 C 7.271606 6.368479 4.994474 4.662668 6.066159

22 C 6.800691 5.727429 4.398538 3.740619 5.010595

23 C 5.355222 4.286075 2.951207 2.398573 3.794040

24 N 4.777601 3.535143 2.419222 1.329321 2.500065

25 Zn 3.389754 3.034126 2.035632 3.031449 4.303421

26 C 3.095003 4.421463 5.398885 6.604518 6.596714

27 H 4.602822 5.724027 6.083971 7.442223 8.001831

28 C 4.972018 3.744469 3.728311 2.641380 1.476421

29 H 2.866030 2.272727 3.332697 3.346676 2.181083

30 C 7.870804 8.251087 7.620823 8.665571 9.927169

31 H 8.367895 8.276562 7.241247 7.901522 9.356103

32 C 8.737940 7.862079 6.487635 6.140804 7.514785

33 H 7.514340 6.349627 5.093457 4.202749 5.261176

34 H 4.150991 5.478482 6.388879 7.631763 7.677267

35 H 3.120937 4.379651 5.460403 6.577949 6.425133

36 H 3.120937 4.379651 5.460403 6.577949 6.425133

37 H 5.566968 4.319038 4.127879 2.947308 2.124126

38 H 5.566968 4.319038 4.127879 2.947308 2.124126

39 H 5.192148 4.116081 4.422961 3.529959 2.120601

40 H 7.865823 8.345010 7.818545 8.920436 10.119703

41 H 7.865823 8.345010 7.818545 8.920436 10.119703

42 H 8.863327 9.165469 8.441630 9.405044 10.727442

43 H 9.103230 8.298113 6.935400 6.688657 8.086081

44 H 9.103230 8.298113 6.935400 6.688657 8.086081

45 H 9.347449 8.367959 7.006745 6.462214 7.728071

11 12 13 14 15

11 C 0.000000

12 N 6.880864 0.000000

13 C 8.476469 2.500065 0.000000

14 C 8.560288 3.555684 1.351884 0.000000

15 C 7.271809 3.535143 2.293729 1.473736 0.000000

16 N 6.297330 2.419222 2.312285 2.295754 1.374500

17 C 7.056635 1.329321 1.501865 2.285284 2.240344

18 N 7.308893 4.777601 3.567094 2.490022 1.327741

19 N 5.015902 5.057611 5.044465 4.444047 2.970347

20 C 6.380966 5.368876 4.684604 3.769001 2.398734

21 C 6.921365 6.817658 6.032009 4.987838 3.741508

22 C 6.023453 7.293332 6.934221 6.042176 4.664656

23 C 4.675082 6.306278 6.401559 5.754886 4.286868

24 N 3.555684 6.833728 7.357884 6.880864 5.409669

25 Zn 4.280144 3.416864 4.303421 4.280144 3.034126

26 C 5.373049 5.027837 7.514785 8.409482 7.862079

27 H 7.078182 2.878225 5.261176 6.419426 6.349627

28 C 2.550589 8.802421 9.927169 9.686249 8.251087

29 H 1.083541 7.592171 9.356103 9.524712 8.276562

30 C 9.686249 3.091433 1.476421 2.550589 3.744469

31 H 9.524712 4.578623 2.181083 1.083541 2.272727

32 C 8.409482 7.811565 6.596714 5.373049 4.421463

33 H 6.419426 8.350817 8.001831 7.078182 5.724027

34 H 6.461719 5.233910 7.728071 8.747005 8.367959

35 H 5.163254 5.639352 8.086081 8.922346 8.298113

36 H 5.163254 5.639352 8.086081 8.922346 8.298113

37 H 3.255857 9.145342 10.119703 9.793881 8.345010

38 H 3.255857 9.145342 10.119703 9.793881 8.345010

39 H 2.706527 9.417461 10.727442 10.575920 9.165469

40 H 9.793881 3.097431 2.124126 3.255857 4.319038

41 H 9.793881 3.097431 2.124126 3.255857 4.319038

42 H 10.575920 4.146982 2.120601 2.706527 4.116081

43 H 8.922346 7.821497 6.425133 5.163254 4.379651

44 H 8.922346 7.821497 6.425133 5.163254 4.379651

45 H 8.747005 8.807994 7.677267 6.461719 5.478482

16 17 18 19 20

16 N 0.000000

17 C 1.358595 0.000000

18 N 2.421152 3.526921 0.000000

19 N 2.888116 4.232934 2.442386 0.000000

20 C 2.964261 4.281717 1.362031 1.365655 0.000000

21 C 4.414452 5.725684 2.499835 2.270611 1.450301

22 C 5.009099 6.366926 3.589161 2.266798 2.275257

23 C 4.232471 5.564356 3.555038 1.358218 2.235300

24 N 5.077881 6.321565 4.848227 2.457652 3.578817

25 Zn 2.035632 3.031449 3.389754 2.033417 3.023478

26 C 6.487635 6.140804 8.737940 7.579008 8.626313

27 H 5.093457 4.202749 7.514340 7.214033 7.866890

28 C 7.620823 8.665571 7.870804 5.431381 6.651164

29 H 7.241247 7.901522 8.367895 6.095887 7.461374

30 C 3.728311 2.641380 4.972018 6.516081 6.142842

31 H 3.332697 3.346676 2.866030 5.134653 4.226779

32 C 5.398885 6.604518 3.095003 3.711869 2.611385

33 H 6.083971 7.442223 4.602822 3.301168 3.326453

34 H 7.006745 6.462214 9.347449 8.400291 9.364862

35 H 6.935400 6.688657 9.103230 7.796438 8.901441

36 H 6.935400 6.688657 9.103230 7.796438 8.901441

37 H 7.818545 8.920436 7.865823 5.471998 6.605901

38 H 7.818545 8.920436 7.865823 5.471998 6.605901

39 H 8.441630 9.405044 8.863327 6.421201 7.677068

40 H 4.127879 2.947308 5.566968 6.943216 6.672806

41 H 4.127879 2.947308 5.566968 6.943216 6.672806

42 H 4.422961 3.529959 5.192148 7.040870 6.471598

43 H 5.460403 6.577949 3.120937 4.136822 2.945397

44 H 5.460403 6.577949 3.120937 4.136822 2.945397

45 H 6.388879 7.631763 4.150991 4.396513 3.493832

21 22 23 24 25

21 C 0.000000

22 C 1.375668 0.000000

23 C 2.274130 1.447424 0.000000

24 N 3.607494 2.511541 1.384417 0.000000

25 Zn 4.251151 4.251507 3.027857 3.416864 0.000000

26 C 9.841311 9.613708 8.202202 7.811565 5.610248

27 H 9.272062 9.468923 8.242479 8.350817 5.228308

28 C 6.645045 5.408272 4.475094 3.091433 5.643122

29 H 7.998098 7.070577 5.743918 4.578623 5.256184

30 C 7.461742 8.401837 7.873946 8.802421 5.643122

31 H 5.237359 6.435254 6.371670 7.592171 5.256184

32 C 1.497643 2.583992 3.742926 5.027837 5.610248

33 H 2.200875 1.077278 2.251177 2.878225 5.228308

34 H 10.639601 10.504249 9.116720 8.807994 6.388453

35 H 10.055833 9.740973 8.316567 7.821497 5.900347

36 H 10.055833 9.740973 8.316567 7.821497 5.900347

37 H 6.462219 5.185490 4.413718 3.097431 5.911068

38 H 6.462219 5.185490 4.413718 3.097431 5.911068

39 H 7.722904 6.495245 5.530805 4.146982 6.424022

40 H 8.016591 8.896221 8.290740 9.145342 5.911068

41 H 8.016591 8.896221 8.290740 9.145342 5.911068

42 H 7.683581 8.746343 8.383445 9.417461 6.424022

43 H 2.157074 3.300341 4.335752 5.639352 5.900347

44 H 2.157074 3.300341 4.335752 5.639352 5.900347

45 H 2.137316 2.726908 4.104377 5.233910 6.388453

26 27 28 29 30

26 C 0.000000

27 H 2.967697 0.000000

28 C 7.923243 9.466110 0.000000

29 H 5.317190 7.414622 2.938850 0.000000

30 C 7.991348 5.362167 11.286244 10.502749 0.000000

31 H 9.483259 7.412741 10.502749 10.512367 2.938850

32 C 11.220497 10.431345 7.991348 9.483259 7.923243

33 H 10.431345 10.456617 5.362167 7.412741 9.466110

34 H 1.089448 2.688949 9.011574 6.394883 8.006613

35 H 1.090848 3.724362 7.682196 4.993521 8.619844

36 H 1.090848 3.724362 7.682196 4.993521 8.619844

37 H 8.539812 9.963034 1.088743 3.690865 11.505900

38 H 8.539812 9.963034 1.088743 3.690865 11.505900

39 H 7.942317 9.784683 1.087952 2.666983 12.043343

40 H 7.739692 5.028898 11.505900 10.560014 1.088743

41 H 7.739692 5.028898 11.505900 10.560014 1.088743

42 H 9.077746 6.439449 12.043343 11.431458 1.087952

43 H 11.462461 10.508460 8.619844 9.997393 7.682196

44 H 11.462461 10.508460 8.619844 9.997393 7.682196

45 H 11.974453 11.360661 8.006613 9.797196 9.011574

31 32 33 34 35

31 H 0.000000

32 C 5.317190 0.000000

33 H 7.414622 2.967697 0.000000

34 H 9.797196 11.974453 11.360661 0.000000

35 H 9.997393 11.462461 10.508460 1.765679 0.000000

36 H 9.997393 11.462461 10.508460 1.765679 1.742927

37 H 10.560014 7.739692 5.028898 9.620609 8.226140

38 H 10.560014 7.739692 5.028898 9.620609 8.408767

39 H 11.431458 9.077746 6.439449 9.027980 7.622320

40 H 3.690865 8.539812 9.963034 7.677889 8.294713

41 H 3.690865 8.539812 9.963034 7.677889 8.475863

42 H 2.666983 7.942317 9.784683 9.091553 9.698687

43 H 4.993521 1.090848 3.724362 12.171081 11.671271

44 H 4.993521 1.090848 3.724362 12.171081 11.800693

45 H 6.394883 1.089448 2.688949 12.776905 12.171081

36 37 38 39 40

36 H 0.000000

37 H 8.408767 0.000000

38 H 8.226140 1.743038 0.000000

39 H 7.622320 1.771588 1.771588 0.000000

40 H 8.475863 11.692934 11.822135 12.217980 0.000000

41 H 8.294713 11.822135 11.692934 12.217980 1.743038

42 H 9.698687 12.217980 12.217980 12.848043 1.771588

43 H 11.800693 8.294713 8.475863 9.698687 8.226140

44 H 11.671271 8.475863 8.294713 9.698687 8.408767

45 H 12.171081 7.677889 7.677889 9.091553 9.620609

41 42 43 44 45

41 H 0.000000

42 H 1.771588 0.000000

43 H 8.408767 7.622320 0.000000

44 H 8.226140 7.622320 1.742927 0.000000

45 H 9.620609 9.027980 1.765679 1.765679 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=3 Diff= 1.83D+00

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 -1.109101 -2.817413 0.000000

2 7 0 -0.000000 -2.033417 0.000000

3 6 0 1.126170 -2.805915 0.000000

4 6 0 0.701975 -4.192793 0.000000

5 6 0 -0.673684 -4.197792 0.000000

6 7 0 2.418339 -2.375303 0.000000

7 6 0 2.823451 -1.110875 0.000000

8 7 0 2.035573 0.015401 0.000000

9 6 0 2.813189 1.129446 0.000000

10 6 0 4.248290 0.686631 0.000000

11 6 0 4.228152 -0.665103 0.000000

12 7 0 -2.429813 -2.402284 0.000000

13 6 0 -4.248290 -0.686631 0.000000

14 6 0 -4.228152 0.665103 0.000000

15 6 0 -2.823451 1.110875 0.000000

16 7 0 -2.035573 -0.015401 0.000000

17 6 0 -2.813189 -1.129446 0.000000

18 7 0 -2.418339 2.375303 0.000000

19 7 0 0.000000 2.033417 0.000000

20 6 0 -1.126170 2.805915 0.000000

21 6 0 -0.701975 4.192793 0.000000

22 6 0 0.673684 4.197792 0.000000

23 6 0 1.109101 2.817413 0.000000

24 7 0 2.429813 2.402284 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 1.630028 -5.368230 0.000000

27 1 0 -1.321467 -5.058551 0.000000

28 6 0 5.413521 1.593305 0.000000

29 1 0 5.085858 -1.327222 0.000000

30 6 0 -5.413521 -1.593305 0.000000

31 1 0 -5.085858 1.327222 0.000000

32 6 0 -1.630028 5.368230 0.000000

33 1 0 1.321467 5.058551 0.000000

34 1 0 1.064167 -6.299197 0.000000

35 1 0 2.286154 -5.369185 0.871463

36 1 0 2.286154 -5.369185 -0.871463

37 1 0 5.397978 2.245664 0.871519

38 1 0 5.397978 2.245664 -0.871519

39 1 0 6.341621 1.025617 0.000000

40 1 0 -5.397978 -2.245664 0.871519

41 1 0 -5.397978 -2.245664 -0.871519

42 1 0 -6.341621 -1.025617 0.000000

43 1 0 -2.286154 5.369185 0.871463

44 1 0 -2.286154 5.369185 -0.871463

45 1 0 -1.064167 6.299197 0.000000

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

Rotational constants (GHZ): 0.1821623 0.1790779 0.0905015

Leave Link 202 at Tue Sep 17 14:05:51 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 101 beta electrons

nuclear repulsion energy 2750.2585778309 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= -0.1138474193 Hartrees.

Nuclear repulsion after empirical dispersion term = 2750.1447304116 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 = 3508

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.12D-07

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 152

GePol: Fraction of low-weight points (<1% of avg) = 4.33%

GePol: Cavity surface area = 383.181 Ang\*\*2

GePol: Cavity volume = 379.658 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0106053310 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2750.1341250806 Hartrees.

Leave Link 301 at Tue Sep 17 14:05:51 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= 15261 LenP2D= 41102.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.87D-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 14:05:52 2019, MaxMem= 2415919104 cpu: 11.8

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:05:52 2019, MaxMem= 2415919104 cpu: 1.3

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= 0.000000 -0.000000 -0.000000

Rot= 0.760836 -0.000000 0.000000 -0.648944 Ang= -80.92 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 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0226 S= 1.0075

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= -1276.15000817517

Leave Link 401 at Tue Sep 17 14:05:54 2019, MaxMem= 2415919104 cpu: 42.3

(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= 36918192.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.11D-15 for 3501.

Iteration 1 A\*A^-1 deviation from orthogonality is 5.60D-15 for 2274 2132.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.66D-15 for 3501.

Iteration 1 A^-1\*A deviation from orthogonality is 5.21D-14 for 2479 2386.

E= -1275.83161712406

DIIS: error= 3.13D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.83161712406 IErMin= 1 ErrMin= 3.13D-03

ErrMax= 3.13D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.01D-02 BMatP= 2.01D-02

IDIUse=3 WtCom= 9.69D-01 WtEn= 3.13D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.303 Goal= None Shift= 0.000

Gap= 0.391 Goal= None Shift= 0.000

GapD= 0.303 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.

RMSDP=2.10D-04 MaxDP=5.78D-03 OVMax= 6.55D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.10D-04 CP: 1.00D+00

E= -1275.83764364577 Delta-E= -0.006026521707 Rises=F Damp=F

DIIS: error= 1.49D-03 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.83764364577 IErMin= 2 ErrMin= 1.49D-03

ErrMax= 1.49D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.49D-03 BMatP= 2.01D-02

IDIUse=3 WtCom= 9.85D-01 WtEn= 1.49D-02

Coeff-Com: 0.135D+00 0.865D+00

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

Coeff: 0.133D+00 0.867D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.079 Goal= None Shift= 0.000

RMSDP=1.10D-04 MaxDP=5.60D-03 DE=-6.03D-03 OVMax= 6.26D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.08D-04 CP: 9.99D-01 1.09D+00

E= -1275.83745146689 Delta-E= 0.000192178881 Rises=F Damp=F

DIIS: error= 2.46D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1275.83764364577 IErMin= 2 ErrMin= 1.49D-03

ErrMax= 2.46D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.19D-03 BMatP= 2.49D-03

IDIUse=3 WtCom= 1.68D-01 WtEn= 8.32D-01

Coeff-Com: -0.133D-01 0.602D+00 0.411D+00

Coeff-En: 0.000D+00 0.551D+00 0.449D+00

Coeff: -0.223D-02 0.560D+00 0.443D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.079 Goal= None Shift= 0.000

RMSDP=6.62D-05 MaxDP=3.37D-03 DE= 1.92D-04 OVMax= 1.12D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 4.92D-05 CP: 9.99D-01 1.19D+00 6.40D-01

E= -1275.83866112496 Delta-E= -0.001209658074 Rises=F Damp=F

DIIS: error= 1.01D-03 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.83866112496 IErMin= 4 ErrMin= 1.01D-03

ErrMax= 1.01D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.39D-04 BMatP= 2.49D-03

IDIUse=3 WtCom= 9.90D-01 WtEn= 1.01D-02

Coeff-Com: -0.101D-01 0.207D+00 0.221D+00 0.583D+00

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

Coeff: -0.100D-01 0.205D+00 0.218D+00 0.587D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=3.59D-05 MaxDP=1.99D-03 DE=-1.21D-03 OVMax= 2.63D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.93D-05 CP: 9.99D-01 1.24D+00 8.88D-01 1.19D+00

E= -1275.83883727496 Delta-E= -0.000176150002 Rises=F Damp=F

DIIS: error= 6.38D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.83883727496 IErMin= 5 ErrMin= 6.38D-04

ErrMax= 6.38D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.16D-04 BMatP= 2.39D-04

IDIUse=3 WtCom= 9.94D-01 WtEn= 6.38D-03

Coeff-Com: -0.104D-02-0.226D-01 0.492D-02 0.414D+00 0.604D+00

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

Coeff: -0.103D-02-0.225D-01 0.489D-02 0.412D+00 0.607D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=3.09D-05 MaxDP=1.47D-03 DE=-1.76D-04 OVMax= 2.33D-02

Cycle 6 Pass 1 IDiag 1:

RMSU= 6.78D-06 CP: 9.99D-01 1.30D+00 1.04D+00 1.62D+00 1.27D+00

E= -1275.83897623326 Delta-E= -0.000138958297 Rises=F Damp=F

DIIS: error= 4.95D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.83897623326 IErMin= 6 ErrMin= 4.95D-04

ErrMax= 4.95D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.71D-05 BMatP= 1.16D-04

IDIUse=3 WtCom= 9.95D-01 WtEn= 4.95D-03

Coeff-Com: 0.766D-02-0.132D+00-0.169D+00-0.960D-01-0.775D-01 0.147D+01

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

Coeff: 0.762D-02-0.132D+00-0.168D+00-0.956D-01-0.771D-01 0.146D+01

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=6.23D-05 MaxDP=3.28D-03 DE=-1.39D-04 OVMax= 4.85D-02

Cycle 7 Pass 1 IDiag 1:

RMSU= 7.91D-06 CP: 9.99D-01 1.41D+00 1.36D+00 2.42D+00 2.30D+00

CP: 2.56D+00

E= -1275.83916783858 Delta-E= -0.000191605326 Rises=F Damp=F

DIIS: error= 3.36D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.83916783858 IErMin= 7 ErrMin= 3.36D-04

ErrMax= 3.36D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.42D-05 BMatP= 4.71D-05

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.36D-03

Coeff-Com: 0.693D-02-0.738D-01-0.152D+00-0.372D+00-0.735D+00 0.131D+01

Coeff-Com: 0.102D+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: 0.690D-02-0.736D-01-0.152D+00-0.371D+00-0.732D+00 0.131D+01

Coeff: 0.102D+01

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=7.03D-05 MaxDP=3.61D-03 DE=-1.92D-04 OVMax= 5.41D-02

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.43D-05 CP: 9.99D-01 1.53D+00 1.71D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.24D+00

E= -1275.83928326634 Delta-E= -0.000115427753 Rises=F Damp=F

DIIS: error= 9.25D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.83928326634 IErMin= 8 ErrMin= 9.25D-05

ErrMax= 9.25D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.06D-06 BMatP= 3.42D-05

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

Coeff-Com: -0.119D-02 0.482D-01 0.295D-01-0.301D-01-0.168D+00-0.118D+00

Coeff-Com: 0.242D+00 0.997D+00

Coeff: -0.119D-02 0.482D-01 0.295D-01-0.301D-01-0.168D+00-0.118D+00

Coeff: 0.242D+00 0.997D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=1.63D-05 MaxDP=8.81D-04 DE=-1.15D-04 OVMax= 1.24D-02

Cycle 9 Pass 1 IDiag 1:

RMSU= 5.20D-06 CP: 9.99D-01 1.56D+00 1.78D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.73D+00 1.48D+00

E= -1275.83929480762 Delta-E= -0.000011541287 Rises=F Damp=F

DIIS: error= 6.93D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.83929480762 IErMin= 9 ErrMin= 6.93D-05

ErrMax= 6.93D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.77D-06 BMatP= 5.06D-06

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

Coeff-Com: -0.240D-02 0.484D-01 0.515D-01 0.568D-01 0.462D-01-0.366D+00

Coeff-Com: -0.886D-01 0.654D+00 0.600D+00

Coeff: -0.240D-02 0.484D-01 0.515D-01 0.568D-01 0.462D-01-0.366D+00

Coeff: -0.886D-01 0.654D+00 0.600D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=8.85D-06 MaxDP=5.21D-04 DE=-1.15D-05 OVMax= 6.74D-03

Cycle 10 Pass 1 IDiag 1:

RMSU= 2.07D-06 CP: 9.99D-01 1.57D+00 1.82D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.98D+00 1.74D+00 1.30D+00

E= -1275.83929856260 Delta-E= -0.000003754972 Rises=F Damp=F

DIIS: error= 3.31D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.83929856260 IErMin=10 ErrMin= 3.31D-05

ErrMax= 3.31D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.44D-07 BMatP= 3.77D-06

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

Coeff-Com: -0.442D-03 0.161D-02 0.879D-02 0.401D-01 0.805D-01-0.107D+00

Coeff-Com: -0.141D+00-0.762D-01 0.283D+00 0.910D+00

Coeff: -0.442D-03 0.161D-02 0.879D-02 0.401D-01 0.805D-01-0.107D+00

Coeff: -0.141D+00-0.762D-01 0.283D+00 0.910D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=4.90D-06 MaxDP=2.66D-04 DE=-3.75D-06 OVMax= 3.70D-03

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.46D-06 CP: 9.99D-01 1.57D+00 1.85D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.88D+00 1.57D+00 1.08D+00

E= -1275.83929961344 Delta-E= -0.000001050844 Rises=F Damp=F

DIIS: error= 1.63D-05 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.83929961344 IErMin=11 ErrMin= 1.63D-05

ErrMax= 1.63D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.48D-07 BMatP= 7.44D-07

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

Coeff-Com: 0.189D-03-0.819D-02-0.600D-02 0.120D-01 0.240D-01 0.158D-01

Coeff-Com: -0.524D-01-0.154D+00 0.345D-01 0.494D+00 0.640D+00

Coeff: 0.189D-03-0.819D-02-0.600D-02 0.120D-01 0.240D-01 0.158D-01

Coeff: -0.524D-01-0.154D+00 0.345D-01 0.494D+00 0.640D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=1.79D-06 MaxDP=9.94D-05 DE=-1.05D-06 OVMax= 1.36D-03

Cycle 12 Pass 1 IDiag 1:

RMSU= 4.86D-07 CP: 9.99D-01 1.58D+00 1.85D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.93D+00 1.64D+00 1.23D+00

CP: 1.28D+00

E= -1275.83929982213 Delta-E= -0.000000208689 Rises=F Damp=F

DIIS: error= 8.80D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.83929982213 IErMin=12 ErrMin= 8.80D-06

ErrMax= 8.80D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.16D-08 BMatP= 2.48D-07

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

Coeff-Com: 0.203D-03-0.379D-02-0.531D-02-0.321D-02-0.155D-01 0.336D-01

Coeff-Com: 0.154D-01-0.457D-01-0.761D-01-0.545D-01 0.288D+00 0.867D+00

Coeff: 0.203D-03-0.379D-02-0.531D-02-0.321D-02-0.155D-01 0.336D-01

Coeff: 0.154D-01-0.457D-01-0.761D-01-0.545D-01 0.288D+00 0.867D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=1.68D-06 MaxDP=8.72D-05 DE=-2.09D-07 OVMax= 1.28D-03

Cycle 13 Pass 1 IDiag 1:

RMSU= 2.94D-07 CP: 9.99D-01 1.58D+00 1.86D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.98D+00 1.72D+00 1.33D+00

CP: 1.59D+00 1.29D+00

E= -1275.83929991400 Delta-E= -0.000000091874 Rises=F Damp=F

DIIS: error= 6.25D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.83929991400 IErMin=13 ErrMin= 6.25D-06

ErrMax= 6.25D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.75D-08 BMatP= 6.16D-08

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

Coeff-Com: 0.591D-04-0.192D-03-0.160D-02-0.315D-02-0.123D-01 0.135D-01

Coeff-Com: 0.182D-01 0.638D-02-0.503D-01-0.145D+00 0.164D-01 0.478D+00

Coeff-Com: 0.679D+00

Coeff: 0.591D-04-0.192D-03-0.160D-02-0.315D-02-0.123D-01 0.135D-01

Coeff: 0.182D-01 0.638D-02-0.503D-01-0.145D+00 0.164D-01 0.478D+00

Coeff: 0.679D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=4.93D-07 MaxDP=2.56D-05 DE=-9.19D-08 OVMax= 3.51D-04

Cycle 14 Pass 1 IDiag 1:

RMSU= 1.25D-07 CP: 9.99D-01 1.58D+00 1.86D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.99D+00 1.74D+00 1.36D+00

CP: 1.71D+00 1.53D+00 1.08D+00

E= -1275.83929992981 Delta-E= -0.000000015802 Rises=F Damp=F

DIIS: error= 2.94D-06 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.83929992981 IErMin=14 ErrMin= 2.94D-06

ErrMax= 2.94D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.98D-09 BMatP= 1.75D-08

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

Coeff-Com: -0.319D-04 0.128D-02 0.888D-03-0.704D-03-0.146D-02-0.419D-02

Coeff-Com: 0.482D-02 0.194D-01-0.204D-03-0.638D-01-0.887D-01-0.402D-01

Coeff-Com: 0.363D+00 0.810D+00

Coeff: -0.319D-04 0.128D-02 0.888D-03-0.704D-03-0.146D-02-0.419D-02

Coeff: 0.482D-02 0.194D-01-0.204D-03-0.638D-01-0.887D-01-0.402D-01

Coeff: 0.363D+00 0.810D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=2.50D-07 MaxDP=1.23D-05 DE=-1.58D-08 OVMax= 1.61D-04

Cycle 15 Pass 1 IDiag 1:

RMSU= 7.58D-08 CP: 9.99D-01 1.58D+00 1.86D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.00D+00 1.75D+00 1.38D+00

CP: 1.78D+00 1.64D+00 1.27D+00 1.33D+00

E= -1275.83929993429 Delta-E= -0.000000004479 Rises=F Damp=F

DIIS: error= 9.27D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.83929993429 IErMin=15 ErrMin= 9.27D-07

ErrMax= 9.27D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.54D-10 BMatP= 3.98D-09

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

Coeff-Com: -0.222D-04 0.329D-03 0.544D-03 0.589D-03 0.240D-02-0.408D-02

Coeff-Com: -0.294D-02 0.274D-02 0.939D-02 0.130D-01-0.186D-01-0.932D-01

Coeff-Com: -0.742D-01 0.152D+00 0.101D+01

Coeff: -0.222D-04 0.329D-03 0.544D-03 0.589D-03 0.240D-02-0.408D-02

Coeff: -0.294D-02 0.274D-02 0.939D-02 0.130D-01-0.186D-01-0.932D-01

Coeff: -0.742D-01 0.152D+00 0.101D+01

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=9.74D-08 MaxDP=6.19D-06 DE=-4.48D-09 OVMax= 5.09D-05

Cycle 16 Pass 1 IDiag 1:

RMSU= 2.94D-08 CP: 9.99D-01 1.58D+00 1.86D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.00D+00 1.76D+00 1.39D+00

CP: 1.81D+00 1.68D+00 1.34D+00 1.65D+00 1.32D+00

E= -1275.83929993505 Delta-E= -0.000000000762 Rises=F Damp=F

DIIS: error= 4.42D-07 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1275.83929993505 IErMin=16 ErrMin= 4.42D-07

ErrMax= 4.42D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.40D-10 BMatP= 5.54D-10

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

Coeff-Com: -0.489D-05-0.176D-03 0.885D-04 0.661D-03 0.197D-02-0.130D-02

Coeff-Com: -0.317D-02-0.414D-02 0.628D-02 0.284D-01 0.151D-01-0.427D-01

Coeff-Com: -0.156D+00-0.148D+00 0.640D+00 0.663D+00

Coeff: -0.489D-05-0.176D-03 0.885D-04 0.661D-03 0.197D-02-0.130D-02

Coeff: -0.317D-02-0.414D-02 0.628D-02 0.284D-01 0.151D-01-0.427D-01

Coeff: -0.156D+00-0.148D+00 0.640D+00 0.663D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=5.03D-08 MaxDP=2.37D-06 DE=-7.62D-10 OVMax= 3.06D-05

Cycle 17 Pass 1 IDiag 1:

RMSU= 1.45D-08 CP: 9.99D-01 1.58D+00 1.86D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.00D+00 1.76D+00 1.39D+00

CP: 1.81D+00 1.69D+00 1.36D+00 1.79D+00 1.60D+00

CP: 1.11D+00

E= -1275.83929993529 Delta-E= -0.000000000239 Rises=F Damp=F

DIIS: error= 2.05D-07 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=17 EnMin= -1275.83929993529 IErMin=17 ErrMin= 2.05D-07

ErrMax= 2.05D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.33D-11 BMatP= 3.40D-10

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

Coeff-Com: 0.430D-06-0.107D-03-0.152D-04 0.203D-03 0.417D-03-0.121D-03

Coeff-Com: -0.754D-03-0.197D-02 0.132D-02 0.102D-01 0.825D-02-0.415D-03

Coeff-Com: -0.543D-01-0.964D-01 0.853D-01 0.280D+00 0.769D+00

Coeff: 0.430D-06-0.107D-03-0.152D-04 0.203D-03 0.417D-03-0.121D-03

Coeff: -0.754D-03-0.197D-02 0.132D-02 0.102D-01 0.825D-02-0.415D-03

Coeff: -0.543D-01-0.964D-01 0.853D-01 0.280D+00 0.769D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=1.71D-08 MaxDP=7.85D-07 DE=-2.39D-10 OVMax= 8.91D-06

Cycle 18 Pass 1 IDiag 1:

RMSU= 7.71D-09 CP: 9.99D-01 1.58D+00 1.86D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.00D+00 1.76D+00 1.39D+00

CP: 1.81D+00 1.69D+00 1.37D+00 1.85D+00 1.68D+00

CP: 1.31D+00 1.06D+00

E= -1275.83929993534 Delta-E= -0.000000000050 Rises=F Damp=F

DIIS: error= 1.07D-07 at cycle 18 NSaved= 18.

NSaved=18 IEnMin=18 EnMin= -1275.83929993534 IErMin=18 ErrMin= 1.07D-07

ErrMax= 1.07D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.84D-11 BMatP= 4.33D-11

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

Coeff-Com: 0.136D-06 0.748D-05 0.504D-05-0.330D-04-0.199D-03 0.615D-04

Coeff-Com: 0.337D-03 0.107D-03-0.606D-03-0.134D-02-0.167D-03 0.965D-02

Coeff-Com: 0.705D-02-0.170D-01-0.107D+00-0.209D-01 0.459D+00 0.671D+00

Coeff: 0.136D-06 0.748D-05 0.504D-05-0.330D-04-0.199D-03 0.615D-04

Coeff: 0.337D-03 0.107D-03-0.606D-03-0.134D-02-0.167D-03 0.965D-02

Coeff: 0.705D-02-0.170D-01-0.107D+00-0.209D-01 0.459D+00 0.671D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=8.66D-09 MaxDP=4.35D-07 DE=-5.00D-11 OVMax= 4.53D-06

Error on total polarization charges = 0.06450

SCF Done: E(UB3LYP) = -1275.83929994 A.U. after 18 cycles

NFock= 18 Conv=0.87D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0188 S= 1.0063

<L.S>= 0.000000000000E+00

KE= 1.320699334188D+03 PE=-8.552090007756D+03 EE= 3.205417248552D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.65

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0188, after 2.0002

Leave Link 502 at Tue Sep 17 14:07:35 2019, MaxMem= 2415919104 cpu: 1770.8

(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= 15261 LenP2D= 41102.

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 14:07:39 2019, MaxMem= 2415919104 cpu: 68.7

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 14:07:39 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 14:07:51 2019, MaxMem= 2415919104 cpu: 230.4

(Enter /home/blab/g09/l716.exe)

Dipole =-1.89626093D-13 4.13891144D-13-4.44089210D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.004220560 0.004558472 -0.000000000

2 7 0.004437851 0.012033011 0.000000000

3 6 -0.001051017 0.012520086 0.000000000

4 6 -0.001612504 -0.016525484 -0.000000000

5 6 0.003447210 0.000477299 0.000000000

6 7 0.005830807 0.000192213 0.000000000

7 6 -0.009911984 0.001616076 0.000000000

8 7 -0.006232153 -0.000028928 -0.000000000

9 6 -0.004307178 0.009931667 -0.000000000

10 6 -0.004403506 -0.004524863 -0.000000000

11 6 0.003891987 -0.002734017 0.000000000

12 7 0.006279954 0.003723269 0.000000000

13 6 0.004403506 0.004524863 -0.000000000

14 6 -0.003891987 0.002734017 0.000000000

15 6 0.009911984 -0.001616076 0.000000000

16 7 0.006232153 0.000028928 0.000000000

17 6 0.004307178 -0.009931667 -0.000000000

18 7 -0.005830807 -0.000192213 0.000000000

19 7 -0.004437851 -0.012033011 -0.000000000

20 6 0.001051017 -0.012520086 -0.000000000

21 6 0.001612504 0.016525484 -0.000000000

22 6 -0.003447210 -0.000477299 0.000000000

23 6 0.004220560 -0.004558472 0.000000000

24 7 -0.006279954 -0.003723269 0.000000000

25 30 0.000000000 0.000000000 0.000000000

26 6 -0.003713193 0.003724617 -0.000000000

27 1 -0.002306868 -0.001158049 -0.000000000

28 6 0.000476523 0.000012642 0.000000000

29 1 -0.001555241 0.000797089 0.000000000

30 6 -0.000476523 -0.000012642 -0.000000000

31 1 0.001555241 -0.000797089 0.000000000

32 6 0.003713193 -0.003724617 0.000000000

33 1 0.002306868 0.001158049 0.000000000

34 1 -0.000593212 -0.001565055 0.000000000

35 1 0.001062354 0.000649595 0.002758546

36 1 0.001062354 0.000649595 -0.002758546

37 1 0.001262334 0.002080976 0.003387395

38 1 0.001262334 0.002080976 -0.003387395

39 1 0.002272372 -0.000684809 0.000000000

40 1 -0.001262334 -0.002080976 0.003387395

41 1 -0.001262334 -0.002080976 -0.003387395

42 1 -0.002272372 0.000684809 -0.000000000

43 1 -0.001062354 -0.000649595 0.002758546

44 1 -0.001062354 -0.000649595 -0.002758546

45 1 0.000593212 0.001565055 0.000000000

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

Cartesian Forces: Max 0.016525484 RMS 0.004135858

Leave Link 716 at Tue Sep 17 14:07:52 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 0.010699520 RMS 0.002330653

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= 2.65D-03 DEPred=-1.63D-03 R=-1.63D+00

Trust test=-1.63D+00 RLast= 2.53D-01 DXMaxT set to 1.26D-01

ITU= -1 0 1 -1 1 1 1 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01332

Eigenvalues --- 0.01333 0.01335 0.01336 0.01347 0.01606

Eigenvalues --- 0.01626 0.01635 0.01644 0.01771 0.01788

Eigenvalues --- 0.01804 0.01812 0.01888 0.01905 0.01941

Eigenvalues --- 0.01946 0.01999 0.02000 0.02047 0.02047

Eigenvalues --- 0.02070 0.02086 0.02101 0.02111 0.02111

Eigenvalues --- 0.02207 0.02315 0.02320 0.02353 0.02375

Eigenvalues --- 0.04836 0.07184 0.07206 0.07251 0.07251

Eigenvalues --- 0.07280 0.07280 0.07390 0.07973 0.12838

Eigenvalues --- 0.14480 0.14493 0.15718 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16003 0.16015

Eigenvalues --- 0.16093 0.16147 0.16324 0.16792 0.21460

Eigenvalues --- 0.22094 0.22125 0.23837 0.23862 0.23907

Eigenvalues --- 0.24375 0.24996 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25004 0.25111

Eigenvalues --- 0.25813 0.26403 0.30374 0.31524 0.33208

Eigenvalues --- 0.33217 0.33248 0.33282 0.33282 0.33380

Eigenvalues --- 0.33707 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33724 0.33949 0.34389 0.34437

Eigenvalues --- 0.34437 0.34437 0.35505 0.35532 0.35554

Eigenvalues --- 0.35614 0.35682 0.35682 0.35691 0.38265

Eigenvalues --- 0.39223 0.40537 0.41642 0.41842 0.43514

Eigenvalues --- 0.48010 0.48989 0.49020 0.49368 0.51284

Eigenvalues --- 0.51347 0.51372 0.53612 0.53922 0.53993

Eigenvalues --- 0.54044 0.56128 0.56331 0.56357

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 0.15795 2.67326 -2.65114 1.05075 -0.23082

Cosine: 0.746 > 0.670

Length: 0.722

GDIIS step was calculated using 5 of the last 10 vectors.

Maximum step size ( 0.126) exceeded in Quadratic search.

-- Step size scaled by 0.560

Iteration 1 RMS(Cart)= 0.01535619 RMS(Int)= 0.00006726

Iteration 2 RMS(Cart)= 0.00012510 RMS(Int)= 0.00001592

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001592

ITry= 1 IFail=0 DXMaxC= 6.16D-02 DCOld= 1.00D+10 DXMaxT= 1.26D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 3.02D-09 for atom 27.

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

(Linear) (Quad) (Total)

R1 2.56666 -0.00142 0.02098 -0.00272 0.01824 2.58490

R2 2.73523 0.00358 -0.00485 0.00214 -0.00268 2.73255

R3 2.61617 -0.00823 -0.02503 0.00364 -0.02139 2.59478

R4 2.58071 -0.00178 -0.01854 0.00170 -0.01686 2.56386

R5 3.84260 -0.00925 -0.02605 -0.00039 -0.02648 3.81612

R6 2.74067 0.00922 0.02340 0.00030 0.02368 2.76435

R7 2.57387 -0.00018 0.00162 0.00194 0.00357 2.57743

R8 2.59964 -0.00063 -0.00276 0.00076 -0.00199 2.59764

R9 2.83014 -0.00394 -0.00997 0.00023 -0.00974 2.82040

R10 2.03576 0.00257 0.00344 0.00011 0.00355 2.03931

R11 2.50907 -0.00595 0.00055 -0.00008 0.00048 2.50955

R12 2.59743 -0.00277 -0.01725 0.00220 -0.01505 2.58238

R13 2.78496 0.00262 0.00853 0.00153 0.01005 2.79501

R14 2.56737 -0.00194 0.01664 -0.00202 0.01467 2.58204

R15 3.84679 -0.01070 -0.03527 -0.00223 -0.03749 3.80930

R16 2.83811 0.00135 -0.00790 0.00389 -0.00400 2.83411

R17 2.51205 -0.00790 -0.01483 0.00247 -0.01233 2.49972

R18 2.55469 0.00028 -0.00155 -0.00054 -0.00209 2.55260

R19 2.79003 0.00604 0.00927 0.00034 0.00961 2.79964

R20 2.04760 -0.00148 -0.00262 0.00008 -0.00254 2.04506

R21 2.51205 -0.00790 -0.01483 0.00247 -0.01233 2.49972

R22 2.55469 0.00028 -0.00155 -0.00054 -0.00209 2.55260

R23 2.83811 0.00135 -0.00790 0.00389 -0.00400 2.83411

R24 2.79003 0.00604 0.00927 0.00034 0.00961 2.79964

R25 2.78496 0.00262 0.00853 0.00153 0.01005 2.79501

R26 2.04760 -0.00148 -0.00262 0.00008 -0.00254 2.04506

R27 2.59743 -0.00277 -0.01725 0.00220 -0.01505 2.58238

R28 2.50907 -0.00595 0.00055 -0.00008 0.00048 2.50955

R29 2.56737 -0.00194 0.01664 -0.00202 0.01467 2.58204

R30 3.84679 -0.01070 -0.03527 -0.00223 -0.03749 3.80930

R31 2.57387 -0.00018 0.00162 0.00194 0.00357 2.57743

R32 2.58071 -0.00178 -0.01854 0.00170 -0.01686 2.56386

R33 2.56666 -0.00142 0.02098 -0.00272 0.01824 2.58490

R34 3.84260 -0.00925 -0.02605 -0.00039 -0.02648 3.81612

R35 2.74067 0.00922 0.02340 0.00030 0.02368 2.76435

R36 2.59964 -0.00063 -0.00276 0.00076 -0.00199 2.59764

R37 2.83014 -0.00394 -0.00997 0.00023 -0.00974 2.82040

R38 2.73523 0.00358 -0.00485 0.00214 -0.00268 2.73255

R39 2.03576 0.00257 0.00344 0.00011 0.00355 2.03931

R40 2.61617 -0.00823 -0.02503 0.00364 -0.02139 2.59478

R41 2.05876 0.00142 0.00149 0.00016 0.00165 2.06041

R42 2.06140 0.00265 0.00329 0.00052 0.00381 2.06522

R43 2.06140 0.00265 0.00329 0.00052 0.00381 2.06522

R44 2.05743 0.00414 0.00450 0.00075 0.00525 2.06267

R45 2.05743 0.00414 0.00450 0.00075 0.00525 2.06267

R46 2.05593 0.00191 0.00251 0.00018 0.00270 2.05863

R47 2.05743 0.00414 0.00450 0.00075 0.00525 2.06267

R48 2.05743 0.00414 0.00450 0.00075 0.00525 2.06267

R49 2.05593 0.00191 0.00251 0.00018 0.00270 2.05863

R50 2.06140 0.00265 0.00329 0.00052 0.00381 2.06522

R51 2.06140 0.00265 0.00329 0.00052 0.00381 2.06522

R52 2.05876 0.00142 0.00149 0.00016 0.00165 2.06041

A1 1.88057 0.00266 0.00385 0.00241 0.00630 1.88686

A2 2.22172 -0.00261 -0.00933 -0.00085 -0.01024 2.21148

A3 2.18089 -0.00005 0.00548 -0.00155 0.00394 2.18484

A4 1.92503 -0.00259 -0.00863 -0.00235 -0.01095 1.91408

A5 2.18612 0.00163 -0.00215 0.00290 0.00069 2.18681

A6 2.17203 0.00096 0.01077 -0.00055 0.01026 2.18229

A7 1.87520 0.00359 0.00987 0.00214 0.01196 1.88717

A8 2.21868 -0.00030 0.00587 -0.00105 0.00484 2.22352

A9 2.18930 -0.00329 -0.01574 -0.00110 -0.01680 2.17249

A10 1.87126 -0.00459 -0.00899 -0.00119 -0.01021 1.86105

A11 2.17644 0.00171 -0.00383 0.00124 -0.00257 2.17386

A12 2.23549 0.00288 0.01281 -0.00005 0.01278 2.24827

A13 1.87272 0.00093 0.00390 -0.00101 0.00290 1.87561

A14 2.19089 -0.00068 -0.00548 0.00044 -0.00505 2.18585

A15 2.21958 -0.00025 0.00159 0.00057 0.00215 2.22173

A16 2.20253 -0.00334 -0.02612 0.00080 -0.02533 2.17719

A17 2.22112 0.00194 0.00644 -0.00006 0.00637 2.22749

A18 2.18815 -0.00244 -0.01275 -0.00033 -0.01308 2.17506

A19 1.87392 0.00050 0.00631 0.00040 0.00671 1.88064

A20 1.92178 0.00105 -0.00507 -0.00065 -0.00573 1.91606

A21 2.17365 0.00084 0.01282 -0.00075 0.01203 2.18568

A22 2.18775 -0.00188 -0.00775 0.00140 -0.00630 2.18145

A23 1.88090 -0.00012 0.00129 0.00095 0.00223 1.88313

A24 2.23965 0.00224 -0.00033 0.00151 0.00123 2.24088

A25 2.16264 -0.00213 -0.00096 -0.00246 -0.00346 2.15918

A26 1.85519 0.00008 0.00141 -0.00074 0.00067 1.85586

A27 2.18105 -0.00352 -0.01080 -0.00134 -0.01215 2.16890

A28 2.24694 0.00345 0.00940 0.00209 0.01148 2.25842

A29 1.89298 -0.00150 -0.00394 0.00005 -0.00389 1.88909

A30 2.17689 -0.00020 -0.00476 -0.00128 -0.00604 2.17085

A31 2.21331 0.00171 0.00870 0.00123 0.00993 2.22324

A32 2.16790 0.00053 0.00978 -0.00335 0.00646 2.17436

A33 1.85519 0.00008 0.00141 -0.00074 0.00067 1.85586

A34 2.24694 0.00345 0.00940 0.00209 0.01148 2.25842

A35 2.18105 -0.00352 -0.01080 -0.00134 -0.01215 2.16890

A36 1.89298 -0.00150 -0.00394 0.00005 -0.00389 1.88909

A37 2.21331 0.00171 0.00870 0.00123 0.00993 2.22324

A38 2.17689 -0.00020 -0.00476 -0.00128 -0.00604 2.17085

A39 1.87392 0.00050 0.00631 0.00040 0.00671 1.88064

A40 2.18815 -0.00244 -0.01275 -0.00033 -0.01308 2.17506

A41 2.22112 0.00194 0.00644 -0.00006 0.00637 2.22749

A42 1.92178 0.00105 -0.00507 -0.00065 -0.00573 1.91606

A43 2.17365 0.00084 0.01282 -0.00075 0.01203 2.18568

A44 2.18775 -0.00188 -0.00775 0.00140 -0.00630 2.18145

A45 2.16264 -0.00213 -0.00096 -0.00246 -0.00346 2.15918

A46 2.23965 0.00224 -0.00033 0.00151 0.00123 2.24088

A47 1.88090 -0.00012 0.00129 0.00095 0.00223 1.88313

A48 2.20253 -0.00334 -0.02612 0.00080 -0.02533 2.17719

A49 1.92503 -0.00259 -0.00863 -0.00235 -0.01095 1.91408

A50 2.17203 0.00096 0.01077 -0.00055 0.01026 2.18229

A51 2.18612 0.00163 -0.00215 0.00290 0.00069 2.18681

A52 2.21868 -0.00030 0.00587 -0.00105 0.00484 2.22352

A53 2.18930 -0.00329 -0.01574 -0.00110 -0.01680 2.17249

A54 1.87520 0.00359 0.00987 0.00214 0.01196 1.88717

A55 1.87126 -0.00459 -0.00899 -0.00119 -0.01021 1.86105

A56 2.17644 0.00171 -0.00383 0.00124 -0.00257 2.17386

A57 2.23549 0.00288 0.01281 -0.00005 0.01278 2.24827

A58 1.87272 0.00093 0.00390 -0.00101 0.00290 1.87561

A59 2.21958 -0.00025 0.00159 0.00057 0.00215 2.22173

A60 2.19089 -0.00068 -0.00548 0.00044 -0.00505 2.18585

A61 1.88057 0.00266 0.00385 0.00241 0.00630 1.88686

A62 2.22172 -0.00261 -0.00933 -0.00085 -0.01024 2.21148

A63 2.18089 -0.00005 0.00548 -0.00155 0.00394 2.18484

A64 2.16790 0.00053 0.00978 -0.00335 0.00646 2.17436

A65 1.57836 -0.00010 -0.00977 0.00160 -0.00816 1.57020

A66 1.56323 0.00010 0.00977 -0.00160 0.00816 1.57139

A67 1.56323 0.00010 0.00977 -0.00160 0.00816 1.57139

A68 1.57836 -0.00010 -0.00977 0.00160 -0.00816 1.57020

A69 1.92711 0.00199 0.00894 0.00056 0.00949 1.93660

A70 1.95348 -0.00194 -0.00686 -0.00040 -0.00725 1.94623

A71 1.95348 -0.00194 -0.00686 -0.00040 -0.00725 1.94623

A72 1.88774 0.00014 0.00113 0.00016 0.00127 1.88901

A73 1.88774 0.00014 0.00113 0.00016 0.00127 1.88901

A74 1.85088 0.00168 0.00263 -0.00006 0.00260 1.85348

A75 1.93552 0.00009 -0.00075 -0.00018 -0.00092 1.93460

A76 1.93552 0.00009 -0.00075 -0.00018 -0.00092 1.93460

A77 1.93139 0.00182 0.00645 0.00098 0.00742 1.93882

A78 1.85620 -0.00013 0.00183 -0.00093 0.00090 1.85709

A79 1.90163 -0.00100 -0.00356 0.00012 -0.00344 1.89819

A80 1.90163 -0.00100 -0.00356 0.00012 -0.00344 1.89819

A81 1.93552 0.00009 -0.00075 -0.00018 -0.00092 1.93460

A82 1.93552 0.00009 -0.00075 -0.00018 -0.00092 1.93460

A83 1.93139 0.00182 0.00645 0.00098 0.00742 1.93882

A84 1.85620 -0.00013 0.00183 -0.00093 0.00090 1.85709

A85 1.90163 -0.00100 -0.00356 0.00012 -0.00344 1.89819

A86 1.90163 -0.00100 -0.00356 0.00012 -0.00344 1.89819

A87 1.95348 -0.00194 -0.00686 -0.00040 -0.00725 1.94623

A88 1.95348 -0.00194 -0.00686 -0.00040 -0.00725 1.94623

A89 1.92711 0.00199 0.00894 0.00056 0.00949 1.93660

A90 1.85088 0.00168 0.00263 -0.00006 0.00260 1.85348

A91 1.88774 0.00014 0.00113 0.00016 0.00127 1.88901

A92 1.88774 0.00014 0.00113 0.00016 0.00127 1.88901

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 1.03758 -0.00025 -0.00289 -0.00032 -0.00323 1.03436

D31 -1.03758 0.00025 0.00289 0.00032 0.00323 -1.03436

D32 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.10401 -0.00025 -0.00289 -0.00032 -0.00323 -2.10724

D34 2.10401 0.00025 0.00289 0.00032 0.00323 2.10724

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 1.02912 -0.00002 0.00066 -0.00069 -0.00003 1.02909

D64 -1.02912 0.00002 -0.00066 0.00069 0.00003 -1.02909

D65 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D66 -2.11247 -0.00002 0.00066 -0.00069 -0.00003 -2.11250

D67 2.11247 0.00002 -0.00066 0.00069 0.00003 2.11250

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 -2.11247 -0.00002 0.00066 -0.00069 -0.00003 -2.11250

D80 2.11247 0.00002 -0.00066 0.00069 0.00003 2.11250

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 1.02912 -0.00002 0.00066 -0.00069 -0.00003 1.02909

D83 -1.02912 0.00002 -0.00066 0.00069 0.00003 -1.02909

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

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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

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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

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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 1.03758 -0.00025 -0.00289 -0.00032 -0.00323 1.03436

D126 -1.03758 0.00025 0.00289 0.00032 0.00323 -1.03436

D127 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D128 -2.10401 -0.00025 -0.00289 -0.00032 -0.00323 -2.10724

D129 2.10401 0.00025 0.00289 0.00032 0.00323 2.10724

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 0.010700 0.000450 NO

RMS Force 0.002331 0.000300 NO

Maximum Displacement 0.061607 0.001800 NO

RMS Displacement 0.015405 0.001200 NO

Predicted change in Energy=-2.846301D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:07:52 2019, MaxMem= 2415919104 cpu: 1.2

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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1 6 0 -2.073499 -2.200384 0.000000

2 7 0 -0.744353 -1.877215 0.000000

3 6 0 0.001212 -3.010733 0.000000

4 6 0 -0.910192 -4.154942 0.000000

5 6 0 -2.185533 -3.642041 0.000000

6 7 0 1.361702 -3.107390 0.000000

7 6 0 2.193971 -2.072546 0.000000

8 7 0 1.873415 -0.744138 0.000000

9 6 0 3.014789 0.006992 0.000000

10 6 0 4.184319 -0.931860 0.000000

11 6 0 3.669080 -2.180508 0.000000

12 7 0 -3.131095 -1.324665 0.000000

13 6 0 -4.184319 0.931860 0.000000

14 6 0 -3.669080 2.180508 0.000000

15 6 0 -2.193971 2.072546 0.000000

16 7 0 -1.873415 0.744138 0.000000

17 6 0 -3.014789 -0.006992 0.000000

18 7 0 -1.361702 3.107390 0.000000

19 7 0 0.744353 1.877215 0.000000

20 6 0 -0.001212 3.010733 0.000000

21 6 0 0.910192 4.154942 0.000000

22 6 0 2.185533 3.642041 0.000000

23 6 0 2.073499 2.200384 0.000000

24 7 0 3.131095 1.324665 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.476118 -5.582914 0.000000

27 1 0 -3.112525 -4.194553 0.000000

28 6 0 5.601279 -0.499328 0.000000

29 1 0 4.213360 -3.115875 0.000000

30 6 0 -5.601279 0.499328 0.000000

31 1 0 -4.213360 3.115875 0.000000

32 6 0 0.476118 5.582914 0.000000

33 1 0 3.112525 4.194553 0.000000

34 1 0 -1.336858 -6.252188 0.000000

35 1 0 0.137604 -5.815184 0.873929

36 1 0 0.137604 -5.815184 -0.873929

37 1 0 5.819199 0.117103 0.874034

38 1 0 5.819199 0.117103 -0.874034

39 1 0 6.272880 -1.357056 0.000000

40 1 0 -5.819199 -0.117103 0.874034

41 1 0 -5.819199 -0.117103 -0.874034

42 1 0 -6.272880 1.357056 0.000000

43 1 0 -0.137604 5.815184 0.873929

44 1 0 -0.137604 5.815184 -0.873929

45 1 0 1.336858 6.252188 0.000000

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Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.367869 0.000000

3 C 2.227351 1.356735 0.000000

4 C 2.274550 2.283756 1.462830 0.000000

5 C 1.446003 2.278510 2.276050 1.374614 0.000000

6 N 3.552923 2.439016 1.363919 2.501773 3.587301

7 C 4.269384 2.944809 2.385034 3.737941 4.652243

8 N 4.206993 2.852469 2.939830 4.402506 4.987274

9 C 5.546457 4.204924 4.264775 5.720767 6.352857

10 C 6.385095 5.018517 4.671199 6.028458 6.922435

11 C 5.742613 4.423841 3.760655 4.986794 6.034283

12 N 1.373096 2.449867 3.557270 3.597621 2.502862

13 C 3.777104 4.441202 5.750019 6.049419 4.991564

14 C 4.662413 5.001914 6.357675 6.910094 6.008576

15 C 4.274628 4.207375 5.537016 6.358435 5.714593

16 N 2.951312 2.854168 4.196818 4.992873 4.397270

17 C 2.386839 2.941533 4.256609 4.651325 3.728438

18 N 5.355290 5.022690 6.268092 7.276355 6.799524

19 N 4.956522 4.038811 4.944118 6.254954 6.248714

20 C 5.608041 4.944118 6.021467 7.223099 7.002190

21 C 7.020868 6.254954 7.223099 8.506937 8.389068

22 C 7.230027 6.248714 7.002190 8.389068 8.494944

23 C 6.046847 4.956522 5.608041 7.020868 7.230027

24 N 6.285998 5.027040 5.347134 6.808678 7.275624

25 Zn 3.023423 2.019406 3.010733 4.253469 4.247472

26 C 3.740740 3.715394 2.616096 1.492489 2.586327

27 H 2.248618 3.313350 3.331184 2.202689 1.079159

28 C 7.861031 6.493506 6.137418 7.467447 8.397088

29 H 6.353166 5.110107 4.213460 5.227852 6.420489

30 C 4.442261 5.407189 6.611236 6.608217 5.368264

31 H 5.730761 6.079882 7.436259 7.985970 7.055602

32 C 8.190255 7.559305 8.606760 9.836041 9.601259

33 H 8.233472 7.193183 7.848338 9.268027 9.459472

34 H 4.118222 4.414912 3.506774 2.140206 2.744653

35 H 4.326604 4.129067 2.940629 2.148960 3.298980

36 H 4.326604 4.129067 2.940629 2.148960 3.298980

37 H 8.272205 6.915306 6.663053 8.018667 8.886554

38 H 8.272205 6.915306 6.663053 8.018667 8.886554

39 H 8.388877 7.036486 6.486021 7.708742 8.761616

40 H 4.374274 5.442058 6.558523 6.416107 5.137378

41 H 4.374274 5.442058 6.558523 6.416107 5.137378

42 H 5.503652 6.405086 7.644725 7.690290 6.457351

43 H 8.292211 7.765623 8.870165 10.038130 9.715805

44 H 8.292211 7.765623 8.870165 10.038130 9.715805

45 H 9.114632 8.391582 9.358721 10.646953 10.502524

6 7 8 9 10

6 N 0.000000

7 C 1.327997 0.000000

8 N 2.418019 1.366537 0.000000

9 C 3.525914 2.235670 1.366356 0.000000

10 C 3.563720 2.294047 2.318516 1.499748 0.000000

11 C 2.486584 1.479055 2.299472 2.283255 1.350776

12 N 4.833563 5.377327 5.038069 6.288497 7.325952

13 C 6.861042 7.050463 6.285310 7.258274 8.573655

14 C 7.298674 7.243192 6.266802 7.028390 8.447645

15 C 6.282877 6.036208 4.947457 5.603364 7.050463

16 N 5.029936 4.947457 4.031588 4.943473 6.285310

17 C 5.363408 5.603364 4.943473 6.029594 7.258274

18 N 6.785310 6.282877 5.029936 5.363408 6.861042

19 N 5.022690 4.207375 2.854168 2.941533 4.441202

20 C 6.268092 5.537016 4.196818 4.256609 5.750019

21 C 7.276355 6.358435 4.992873 4.651325 6.049419

22 C 6.799524 5.714593 4.397270 3.728438 4.991564

23 C 5.355290 4.274628 2.951312 2.386839 3.777104

24 N 4.772198 3.524095 2.421095 1.322797 2.490218

25 Zn 3.392655 3.018104 2.015794 3.014797 4.286828

26 C 3.083148 4.410449 5.379040 6.590408 6.584222

27 H 4.604414 5.715051 6.063412 7.429465 7.993066

28 C 4.977550 3.752967 3.735893 2.635582 1.481505

29 H 2.851670 2.272987 3.331738 3.344977 2.184209

30 C 7.841653 8.208560 7.577418 8.630123 9.889704

31 H 8.355259 8.244610 7.207533 7.868373 9.322295

32 C 8.735311 7.845832 6.479508 6.126643 7.496202

33 H 7.508912 6.334056 5.091763 4.188701 5.237256

34 H 4.143909 5.471395 6.375302 7.623265 7.667418

35 H 3.097469 4.358869 5.430681 6.552837 6.402071

36 H 3.097469 4.358869 5.430681 6.552837 6.402071

37 H 5.570510 4.324440 4.132176 2.939520 2.130045

38 H 5.570510 4.324440 4.132176 2.939520 2.130045

39 H 5.213765 4.141187 4.441955 3.532108 2.131403

40 H 7.827586 8.294491 7.767460 8.877989 10.074629

41 H 7.827586 8.294491 7.767460 8.877989 10.074629

42 H 8.844101 9.135082 8.412916 9.385280 10.704773

43 H 9.089774 8.271412 6.916115 6.666065 8.060110

44 H 9.089774 8.271412 6.916115 6.666065 8.060110

45 H 9.359612 8.368742 7.016870 6.466679 7.727780

11 12 13 14 15

11 C 0.000000

12 N 6.853819 0.000000

13 C 8.447645 2.490218 0.000000

14 C 8.536220 3.546219 1.350776 0.000000

15 C 7.243192 3.524095 2.294047 1.479055 0.000000

16 N 6.266802 2.421095 2.318516 2.299472 1.366537

17 C 7.028390 1.322797 1.499748 2.283255 2.235670

18 N 7.298674 4.772198 3.563720 2.486584 1.327997

19 N 5.001914 5.027040 5.018517 4.423841 2.944809

20 C 6.357675 5.347134 4.671199 3.760655 2.385034

21 C 6.910094 6.808678 6.028458 4.986794 3.737941

22 C 6.008576 7.275624 6.922435 6.034283 4.652243

23 C 4.662413 6.285998 6.385095 5.742613 4.269384

24 N 3.546219 6.799557 7.325952 6.853819 5.377327

25 Zn 4.268110 3.399778 4.286828 4.268110 3.018104

26 C 5.362744 5.018126 7.496202 8.394387 7.845832

27 H 7.074357 2.869948 5.237256 6.399309 6.334056

28 C 2.561203 8.771290 9.889704 9.649926 8.208560

29 H 1.082198 7.559725 9.322295 9.496554 8.244610

30 C 9.649926 3.070629 1.481505 2.561203 3.752967

31 H 9.496554 4.570525 2.184209 1.082198 2.272987

32 C 8.394387 7.792730 6.584222 5.362744 4.410449

33 H 6.399309 8.333340 7.993066 7.074357 5.715051

34 H 6.452750 5.244022 7.727780 8.749265 8.368742

35 H 5.142561 5.622535 8.060110 8.898634 8.271412

36 H 5.142561 5.622535 8.060110 8.898634 8.271412

37 H 3.265880 9.107711 10.074629 9.749308 8.294491

38 H 3.265880 9.107711 10.074629 9.749308 8.294491

39 H 2.730907 9.404031 10.704773 10.552579 9.135082

40 H 9.749308 3.073768 2.130045 3.265880 4.324440

41 H 9.749308 3.073768 2.130045 3.265880 4.324440

42 H 10.552579 4.130671 2.131403 2.730907 4.141187

43 H 8.898634 7.791161 6.402071 5.142561 4.358869

44 H 8.898634 7.791161 6.402071 5.142561 4.358869

45 H 8.749265 8.796096 7.667418 6.452750 5.471395

16 17 18 19 20

16 N 0.000000

17 C 1.366356 0.000000

18 N 2.418019 3.525914 0.000000

19 N 2.852469 4.204924 2.439016 0.000000

20 C 2.939830 4.264775 1.363919 1.356735 0.000000

21 C 4.402506 5.720767 2.501773 2.283756 1.462830

22 C 4.987274 6.352857 3.587301 2.278510 2.276050

23 C 4.206993 5.546457 3.552923 1.367869 2.227351

24 N 5.038069 6.288497 4.833563 2.449867 3.557270

25 Zn 2.015794 3.014797 3.392655 2.019406 3.010733

26 C 6.479508 6.126643 8.735311 7.559305 8.606760

27 H 5.091763 4.188701 7.508912 7.193183 7.848338

28 C 7.577418 8.630123 7.841653 5.407189 6.611236

29 H 7.207533 7.868373 8.355259 6.079882 7.436259

30 C 3.735893 2.635582 4.977550 6.493506 6.137418

31 H 3.331738 3.344977 2.851670 5.110107 4.213460

32 C 5.379040 6.590408 3.083148 3.715394 2.616096

33 H 6.063412 7.429465 4.604414 3.313350 3.331184

34 H 7.016870 6.466679 9.359612 8.391582 9.358721

35 H 6.916115 6.666065 9.089774 7.765623 8.870165

36 H 6.916115 6.666065 9.089774 7.765623 8.870165

37 H 7.767460 8.877989 7.827586 5.442058 6.558523

38 H 7.767460 8.877989 7.827586 5.442058 6.558523

39 H 8.412916 9.385280 8.844101 6.405086 7.644725

40 H 4.132176 2.939520 5.570510 6.915306 6.663053

41 H 4.132176 2.939520 5.570510 6.915306 6.663053

42 H 4.441955 3.532108 5.213765 7.036486 6.486021

43 H 5.430681 6.552837 3.097469 4.129067 2.940629

44 H 5.430681 6.552837 3.097469 4.129067 2.940629

45 H 6.375302 7.623265 4.143909 4.414912 3.506774

21 22 23 24 25

21 C 0.000000

22 C 1.374614 0.000000

23 C 2.274550 1.446003 0.000000

24 N 3.597621 2.502862 1.373096 0.000000

25 Zn 4.253469 4.247472 3.023423 3.399778 0.000000

26 C 9.836041 9.601259 8.190255 7.792730 5.603179

27 H 9.268027 9.459472 8.233472 8.333340 5.223225

28 C 6.608217 5.368264 4.442261 3.070629 5.623491

29 H 7.985970 7.055602 5.730761 4.570525 5.240332

30 C 7.467447 8.397088 7.861031 8.771290 5.623491

31 H 5.227852 6.420489 6.353166 7.559725 5.240332

32 C 1.492489 2.586327 3.740740 5.018126 5.603179

33 H 2.202689 1.079159 2.248618 2.869948 5.223225

34 H 10.646953 10.502524 9.114632 8.796096 6.393516

35 H 10.038130 9.715805 8.292211 7.791161 5.882095

36 H 10.038130 9.715805 8.292211 7.791161 5.882095

37 H 6.416107 5.137378 4.374274 3.073768 5.885638

38 H 6.416107 5.137378 4.374274 3.073768 5.885638

39 H 7.690290 6.457351 5.503652 4.130671 6.417993

40 H 8.018667 8.886554 8.272205 9.107711 5.885638

41 H 8.018667 8.886554 8.272205 9.107711 5.885638

42 H 7.708742 8.761616 8.388877 9.404031 6.417993

43 H 2.148960 3.298980 4.326604 5.622535 5.882095

44 H 2.148960 3.298980 4.326604 5.622535 5.882095

45 H 2.140206 2.744653 4.118222 5.244022 6.393516

26 27 28 29 30

26 C 0.000000

27 H 2.979629 0.000000

28 C 7.923232 9.464939 0.000000

29 H 5.298819 7.404872 2.961864 0.000000

30 C 7.953675 5.312854 11.246983 10.459294 0.000000

31 H 9.467625 7.392848 10.459294 10.480664 2.961864

32 C 11.206359 10.415240 7.953675 9.467625 7.923232

33 H 10.415240 10.446451 5.312854 7.392848 9.464939

34 H 1.090321 2.717877 9.012943 6.375059 7.985503

35 H 1.092866 3.735443 7.672928 4.966065 8.577388

36 H 1.092866 3.735443 7.672928 4.966065 8.577388

37 H 8.537280 9.956405 1.091518 3.714136 11.460251

38 H 8.537280 9.956405 1.091518 3.714136 11.460251

39 H 7.962842 9.804959 1.089378 2.708334 12.018395

40 H 7.693344 4.971480 11.460251 10.507560 1.091518

41 H 7.693344 4.971480 11.460251 10.507560 1.091518

42 H 9.042436 6.388130 12.018395 11.400366 1.089378

43 H 11.436563 10.478966 8.577388 9.972886 7.672928

44 H 11.436563 10.478966 8.577388 9.972886 7.672928

45 H 11.973159 11.354797 7.985503 9.799739 9.012943

31 32 33 34 35

31 H 0.000000

32 C 5.298819 0.000000

33 H 7.404872 2.979629 0.000000

34 H 9.799739 11.973159 11.354797 0.000000

35 H 9.972886 11.436563 10.478966 1.768831 0.000000

36 H 9.972886 11.436563 10.478966 1.768831 1.747858

37 H 10.507560 7.693344 4.971480 9.619821 8.214168

38 H 10.507560 7.693344 4.971480 9.619821 8.398091

39 H 11.400366 9.042436 6.388130 9.048228 7.634152

40 H 3.714136 8.537280 9.956405 7.648176 8.243278

41 H 3.714136 8.537280 9.956405 7.648176 8.426565

42 H 2.708334 7.962842 9.804959 9.070001 9.659145

43 H 4.966065 1.092866 3.735443 12.158266 11.633623

44 H 4.966065 1.092866 3.735443 12.158266 11.764191

45 H 6.375059 1.090321 2.717877 12.787032 12.158266

36 37 38 39 40

36 H 0.000000

37 H 8.398091 0.000000

38 H 8.214168 1.748068 0.000000

39 H 7.634152 1.772825 1.772825 0.000000

40 H 8.426565 11.640755 11.771275 12.186870 0.000000

41 H 8.243278 11.771275 11.640755 12.186870 1.748068

42 H 9.659145 12.186870 12.186870 12.835985 1.772825

43 H 11.764191 8.243278 8.426565 9.659145 8.214168

44 H 11.633623 8.426565 8.243278 9.659145 8.398091

45 H 12.158266 7.648176 7.648176 9.070001 9.619821

41 42 43 44 45

41 H 0.000000

42 H 1.772825 0.000000

43 H 8.398091 7.634152 0.000000

44 H 8.214168 7.634152 1.747858 0.000000

45 H 9.619821 9.048228 1.768831 1.768831 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=0 Diff= 2.00D+00

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 2.810407 -1.114765 0.000000

2 7 0 2.019405 0.001203 0.000000

3 6 0 2.797633 1.112549 0.000000

4 6 0 4.197473 0.687908 0.000000

5 6 0 4.191595 -0.686693 0.000000

6 7 0 2.385233 2.412627 0.000000

7 6 0 1.116246 2.804094 0.000000

8 7 0 0.000000 2.015794 0.000000

9 6 0 -1.119418 2.799268 0.000000

10 6 0 -0.678615 4.232774 0.000000

11 6 0 0.672042 4.214869 0.000000

12 7 0 2.386957 -2.420936 0.000000

13 6 0 0.678615 -4.232774 0.000000

14 6 0 -0.672042 -4.214869 0.000000

15 6 0 -1.116246 -2.804094 0.000000

16 7 0 -0.000000 -2.015794 0.000000

17 6 0 1.119418 -2.799268 0.000000

18 7 0 -2.385233 -2.412627 0.000000

19 7 0 -2.019405 -0.001203 0.000000

20 6 0 -2.797633 -1.112549 0.000000

21 6 0 -4.197473 -0.687908 0.000000

22 6 0 -4.191595 0.686693 0.000000

23 6 0 -2.810407 1.114765 0.000000

24 7 0 -2.386957 2.420936 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 5.364345 1.618464 0.000000

27 1 0 5.047285 -1.344248 0.000000

28 6 0 -1.603672 5.389981 0.000000

29 1 0 1.340420 5.066000 0.000000

30 6 0 1.603672 -5.389981 0.000000

31 1 0 -1.340420 -5.066000 0.000000

32 6 0 -5.364345 -1.618464 0.000000

33 1 0 -5.047285 1.344248 0.000000

34 1 0 6.304092 1.065584 0.000000

35 1 0 5.353651 2.274580 0.873929

36 1 0 5.353651 2.274580 -0.873929

37 1 0 -2.257010 5.364951 0.874034

38 1 0 -2.257010 5.364951 -0.874034

39 1 0 -1.054451 6.330779 0.000000

40 1 0 2.257010 -5.364951 0.874034

41 1 0 2.257010 -5.364951 -0.874034

42 1 0 1.054451 -6.330779 0.000000

43 1 0 -5.353651 -2.274580 0.873929

44 1 0 -5.353651 -2.274580 -0.873929

45 1 0 -6.304092 -1.065584 0.000000

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

Rotational constants (GHZ): 0.1825266 0.1806272 0.0909873

Leave Link 202 at Tue Sep 17 14:07:52 2019, MaxMem= 2415919104 cpu: 0.1

(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 101 beta electrons

nuclear repulsion energy 2756.2713087063 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= -0.1140573895 Hartrees.

Nuclear repulsion after empirical dispersion term = 2756.1572513168 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 = 3496

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.96D-08

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 124

GePol: Fraction of low-weight points (<1% of avg) = 3.55%

GePol: Cavity surface area = 382.506 Ang\*\*2

GePol: Cavity volume = 379.326 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0106456388 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2756.1466056780 Hartrees.

Leave Link 301 at Tue Sep 17 14:07:52 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= 15297 LenP2D= 41162.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.86D-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 14:07:52 2019, MaxMem= 2415919104 cpu: 10.7

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:07:52 2019, MaxMem= 2415919104 cpu: 1.2

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= -0.000000 0.000000 0.000000

Rot= 0.707538 0.000000 0.000000 -0.706676 Ang= -89.93 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 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0188 S= 1.0063

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= -1276.15053097663

Leave Link 401 at Tue Sep 17 14:07:55 2019, MaxMem= 2415919104 cpu: 39.7

(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= 36666048.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.99D-15 for 3496.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.18D-15 for 3137 3063.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.33D-15 for 3496.

Iteration 1 A^-1\*A deviation from orthogonality is 7.94D-12 for 1904 1857.

E= -1275.84023364763

DIIS: error= 1.82D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.84023364763 IErMin= 1 ErrMin= 1.82D-03

ErrMax= 1.82D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.18D-03 BMatP= 5.18D-03

IDIUse=3 WtCom= 9.82D-01 WtEn= 1.82D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.303 Goal= None Shift= 0.000

Gap= 0.392 Goal= None Shift= 0.000

GapD= 0.303 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.

RMSDP=1.01D-04 MaxDP=2.13D-03 OVMax= 2.22D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.01D-04 CP: 1.00D+00

E= -1275.84169913575 Delta-E= -0.001465488113 Rises=F Damp=F

DIIS: error= 6.46D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84169913575 IErMin= 2 ErrMin= 6.46D-04

ErrMax= 6.46D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.49D-04 BMatP= 5.18D-03

IDIUse=3 WtCom= 9.94D-01 WtEn= 6.46D-03

Coeff-Com: 0.113D+00 0.887D+00

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

Coeff: 0.113D+00 0.887D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=4.90D-05 MaxDP=2.40D-03 DE=-1.47D-03 OVMax= 2.65D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 4.87D-05 CP: 1.00D+00 1.06D+00

E= -1275.84162768243 Delta-E= 0.000071453316 Rises=F Damp=F

DIIS: error= 1.15D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1275.84169913575 IErMin= 2 ErrMin= 6.46D-04

ErrMax= 1.15D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.20D-03 BMatP= 5.49D-04

IDIUse=3 WtCom= 2.28D-01 WtEn= 7.72D-01

Coeff-Com: -0.152D-01 0.608D+00 0.407D+00

Coeff-En: 0.000D+00 0.585D+00 0.415D+00

Coeff: -0.346D-02 0.591D+00 0.413D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=2.85D-05 MaxDP=1.35D-03 DE= 7.15D-05 OVMax= 5.30D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.02D-05 CP: 1.00D+00 1.13D+00 6.15D-01

E= -1275.84189715482 Delta-E= -0.000269472393 Rises=F Damp=F

DIIS: error= 3.34D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84189715482 IErMin= 4 ErrMin= 3.34D-04

ErrMax= 3.34D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.96D-05 BMatP= 5.49D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.34D-03

Coeff-Com: -0.976D-02 0.212D+00 0.180D+00 0.617D+00

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

Coeff: -0.973D-02 0.212D+00 0.180D+00 0.618D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=1.41D-05 MaxDP=7.39D-04 DE=-2.69D-04 OVMax= 1.02D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 8.21D-06 CP: 1.00D+00 1.16D+00 8.17D-01 1.24D+00

E= -1275.84192387190 Delta-E= -0.000026717077 Rises=F Damp=F

DIIS: error= 2.59D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84192387190 IErMin= 5 ErrMin= 2.59D-04

ErrMax= 2.59D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.03D-05 BMatP= 2.96D-05

IDIUse=3 WtCom= 9.97D-01 WtEn= 2.59D-03

Coeff-Com: -0.156D-02-0.109D-01-0.580D-02 0.433D+00 0.585D+00

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

Coeff: -0.156D-02-0.109D-01-0.578D-02 0.432D+00 0.587D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=1.20D-05 MaxDP=5.45D-04 DE=-2.67D-05 OVMax= 8.85D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.84D-06 CP: 1.00D+00 1.20D+00 9.49D-01 1.67D+00 1.26D+00

E= -1275.84194651348 Delta-E= -0.000022641576 Rises=F Damp=F

DIIS: error= 1.99D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84194651348 IErMin= 6 ErrMin= 1.99D-04

ErrMax= 1.99D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.75D-06 BMatP= 2.03D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.99D-03

Coeff-Com: 0.648D-02-0.124D+00-0.143D+00-0.120D+00-0.851D-01 0.146D+01

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

Coeff: 0.646D-02-0.123D+00-0.142D+00-0.120D+00-0.849D-01 0.146D+01

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=2.50D-05 MaxDP=1.26D-03 DE=-2.26D-05 OVMax= 1.92D-02

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.79D-06 CP: 1.00D+00 1.27D+00 1.24D+00 2.50D+00 2.30D+00

CP: 2.34D+00

E= -1275.84197851127 Delta-E= -0.000031997790 Rises=F Damp=F

DIIS: error= 1.40D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84197851127 IErMin= 7 ErrMin= 1.40D-04

ErrMax= 1.40D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.97D-06 BMatP= 7.75D-06

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.40D-03

Coeff-Com: 0.674D-02-0.883D-01-0.133D+00-0.419D+00-0.718D+00 0.131D+01

Coeff-Com: 0.104D+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: 0.673D-02-0.882D-01-0.133D+00-0.418D+00-0.717D+00 0.131D+01

Coeff: 0.104D+01

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=3.06D-05 MaxDP=1.53D-03 DE=-3.20D-05 OVMax= 2.35D-02

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.24D-05 CP: 1.00D+00 1.35D+00 1.59D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.97D+00

E= -1275.84199963738 Delta-E= -0.000021126114 Rises=F Damp=F

DIIS: error= 4.32D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84199963738 IErMin= 8 ErrMin= 4.32D-05

ErrMax= 4.32D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.02D-06 BMatP= 5.97D-06

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

Coeff-Com: 0.102D-05 0.258D-01 0.433D-02-0.628D-01-0.249D+00-0.345D-01

Coeff-Com: 0.379D+00 0.937D+00

Coeff: 0.102D-05 0.258D-01 0.433D-02-0.628D-01-0.249D+00-0.345D-01

Coeff: 0.379D+00 0.937D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=9.93D-06 MaxDP=5.29D-04 DE=-2.11D-05 OVMax= 7.72D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.99D-06 CP: 1.00D+00 1.38D+00 1.70D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.60D+00 1.61D+00

E= -1275.84200220222 Delta-E= -0.000002564844 Rises=F Damp=F

DIIS: error= 2.28D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84200220222 IErMin= 9 ErrMin= 2.28D-05

ErrMax= 2.28D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.57D-07 BMatP= 1.02D-06

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

Coeff-Com: -0.179D-02 0.407D-01 0.351D-01 0.671D-01 0.211D-01-0.340D+00

Coeff-Com: -0.341D-01 0.598D+00 0.614D+00

Coeff: -0.179D-02 0.407D-01 0.351D-01 0.671D-01 0.211D-01-0.340D+00

Coeff: -0.341D-01 0.598D+00 0.614D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=2.89D-06 MaxDP=1.61D-04 DE=-2.56D-06 OVMax= 2.18D-03

Cycle 10 Pass 1 IDiag 1:

RMSU= 8.19D-07 CP: 1.00D+00 1.38D+00 1.72D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.83D+00 1.79D+00 1.16D+00

E= -1275.84200270281 Delta-E= -0.000000500588 Rises=F Damp=F

DIIS: error= 1.00D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84200270281 IErMin=10 ErrMin= 1.00D-05

ErrMax= 1.00D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.31D-08 BMatP= 5.57D-07

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

Coeff-Com: -0.412D-03 0.211D-02 0.558D-02 0.439D-01 0.935D-01-0.810D-01

Coeff-Com: -0.155D+00-0.117D+00 0.201D+00 0.101D+01

Coeff: -0.412D-03 0.211D-02 0.558D-02 0.439D-01 0.935D-01-0.810D-01

Coeff: -0.155D+00-0.117D+00 0.201D+00 0.101D+01

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=1.65D-06 MaxDP=9.13D-05 DE=-5.01D-07 OVMax= 1.20D-03

Cycle 11 Pass 1 IDiag 1:

RMSU= 5.18D-07 CP: 1.00D+00 1.39D+00 1.74D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.87D+00 1.37D+00 1.53D+00

E= -1275.84200287598 Delta-E= -0.000000173168 Rises=F Damp=F

DIIS: error= 7.52D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84200287598 IErMin=11 ErrMin= 7.52D-06

ErrMax= 7.52D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.10D-08 BMatP= 9.31D-08

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

Coeff-Com: 0.831D-04-0.755D-02-0.498D-02 0.168D-01 0.500D-01 0.281D-01

Coeff-Com: -0.927D-01-0.209D+00-0.406D-01 0.600D+00 0.659D+00

Coeff: 0.831D-04-0.755D-02-0.498D-02 0.168D-01 0.500D-01 0.281D-01

Coeff: -0.927D-01-0.209D+00-0.406D-01 0.600D+00 0.659D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=7.48D-07 MaxDP=3.94D-05 DE=-1.73D-07 OVMax= 5.25D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 2.95D-07 CP: 1.00D+00 1.39D+00 1.75D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.91D+00 1.44D+00 1.84D+00

CP: 1.31D+00

E= -1275.84200292466 Delta-E= -0.000000048683 Rises=F Damp=F

DIIS: error= 4.14D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84200292466 IErMin=12 ErrMin= 4.14D-06

ErrMax= 4.14D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.31D-08 BMatP= 5.10D-08

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

Coeff-Com: 0.202D-03-0.410D-02-0.510D-02-0.632D-02-0.203D-01 0.422D-01

Coeff-Com: 0.154D-01-0.419D-01-0.934D-01-0.954D-01 0.279D+00 0.930D+00

Coeff: 0.202D-03-0.410D-02-0.510D-02-0.632D-02-0.203D-01 0.422D-01

Coeff: 0.154D-01-0.419D-01-0.934D-01-0.954D-01 0.279D+00 0.930D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=8.70D-07 MaxDP=4.70D-05 DE=-4.87D-08 OVMax= 6.67D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.77D-07 CP: 1.00D+00 1.39D+00 1.76D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.96D+00 1.52D+00 2.00D+00

CP: 1.58D+00 1.44D+00

E= -1275.84200294827 Delta-E= -0.000000023607 Rises=F Damp=F

DIIS: error= 2.08D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84200294827 IErMin=13 ErrMin= 2.08D-06

ErrMax= 2.08D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.07D-09 BMatP= 1.31D-08

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

Coeff-Com: 0.102D-03-0.780D-03-0.207D-02-0.683D-02-0.241D-01 0.179D-01

Coeff-Com: 0.291D-01 0.245D-01-0.461D-01-0.201D+00-0.215D-02 0.558D+00

Coeff-Com: 0.654D+00

Coeff: 0.102D-03-0.780D-03-0.207D-02-0.683D-02-0.241D-01 0.179D-01

Coeff: 0.291D-01 0.245D-01-0.461D-01-0.201D+00-0.215D-02 0.558D+00

Coeff: 0.654D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=3.65D-07 MaxDP=1.89D-05 DE=-2.36D-08 OVMax= 2.79D-04

Cycle 14 Pass 1 IDiag 1:

RMSU= 5.68D-08 CP: 1.00D+00 1.39D+00 1.76D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.99D+00 1.55D+00 2.06D+00

CP: 1.68D+00 1.72D+00 1.20D+00

E= -1275.84200295241 Delta-E= -0.000000004140 Rises=F Damp=F

DIIS: error= 8.68D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84200295241 IErMin=14 ErrMin= 8.68D-07

ErrMax= 8.68D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.20D-10 BMatP= 4.07D-09

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

Coeff-Com: -0.127D-04 0.105D-02 0.677D-03-0.777D-03-0.529D-02-0.578D-02

Coeff-Com: 0.865D-02 0.261D-01 0.756D-02-0.781D-01-0.911D-01 0.241D-01

Coeff-Com: 0.324D+00 0.789D+00

Coeff: -0.127D-04 0.105D-02 0.677D-03-0.777D-03-0.529D-02-0.578D-02

Coeff: 0.865D-02 0.261D-01 0.756D-02-0.781D-01-0.911D-01 0.241D-01

Coeff: 0.324D+00 0.789D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=1.44D-07 MaxDP=7.52D-06 DE=-4.14D-09 OVMax= 1.08D-04

Cycle 15 Pass 1 IDiag 1:

RMSU= 2.58D-08 CP: 1.00D+00 1.39D+00 1.76D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.99D+00 1.56D+00 2.09D+00

CP: 1.73D+00 1.83D+00 1.37D+00 1.07D+00

E= -1275.84200295298 Delta-E= -0.000000000568 Rises=F Damp=F

DIIS: error= 2.68D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.84200295298 IErMin=15 ErrMin= 2.68D-07

ErrMax= 2.68D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.21D-10 BMatP= 6.20D-10

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

Coeff-Com: -0.127D-04 0.569D-03 0.479D-03-0.263D-03-0.118D-02-0.400D-02

Coeff-Com: 0.297D-02 0.118D-01 0.814D-02-0.255D-01-0.473D-01-0.345D-01

Coeff-Com: 0.896D-01 0.382D+00 0.617D+00

Coeff: -0.127D-04 0.569D-03 0.479D-03-0.263D-03-0.118D-02-0.400D-02

Coeff: 0.297D-02 0.118D-01 0.814D-02-0.255D-01-0.473D-01-0.345D-01

Coeff: 0.896D-01 0.382D+00 0.617D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=3.19D-08 MaxDP=1.51D-06 DE=-5.68D-10 OVMax= 2.24D-05

Cycle 16 Pass 1 IDiag 1:

RMSU= 9.56D-09 CP: 1.00D+00 1.39D+00 1.76D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.00D+00 1.56D+00 2.09D+00

CP: 1.73D+00 1.85D+00 1.40D+00 1.19D+00 1.03D+00

E= -1275.84200295300 Delta-E= -0.000000000019 Rises=F Damp=F

DIIS: error= 1.71D-07 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1275.84200295300 IErMin=16 ErrMin= 1.71D-07

ErrMax= 1.71D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.91D-11 BMatP= 1.21D-10

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

Coeff-Com: -0.305D-05-0.904D-04 0.367D-04 0.292D-03 0.181D-02-0.942D-04

Coeff-Com: -0.201D-02-0.426D-02 0.199D-02 0.152D-01 0.701D-02-0.244D-01

Coeff-Com: -0.639D-01-0.574D-01 0.354D+00 0.772D+00

Coeff: -0.305D-05-0.904D-04 0.367D-04 0.292D-03 0.181D-02-0.942D-04

Coeff: -0.201D-02-0.426D-02 0.199D-02 0.152D-01 0.701D-02-0.244D-01

Coeff: -0.639D-01-0.574D-01 0.354D+00 0.772D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=2.21D-08 MaxDP=1.11D-06 DE=-1.91D-11 OVMax= 1.62D-05

Cycle 17 Pass 1 IDiag 1:

RMSU= 6.42D-09 CP: 1.00D+00 1.39D+00 1.76D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.99D+00 1.56D+00 2.09D+00

CP: 1.74D+00 1.85D+00 1.39D+00 1.21D+00 1.23D+00

CP: 1.15D+00

E= -1275.84200295303 Delta-E= -0.000000000032 Rises=F Damp=F

DIIS: error= 7.95D-08 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=17 EnMin= -1275.84200295303 IErMin=17 ErrMin= 7.95D-08

ErrMax= 7.95D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.47D-12 BMatP= 3.91D-11

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

Coeff-Com: 0.762D-06-0.988D-04-0.411D-04 0.122D-03 0.687D-03 0.518D-03

Coeff-Com: -0.914D-03-0.291D-02-0.372D-03 0.866D-02 0.885D-02-0.247D-02

Coeff-Com: -0.298D-01-0.748D-01-0.287D-02 0.248D+00 0.848D+00

Coeff: 0.762D-06-0.988D-04-0.411D-04 0.122D-03 0.687D-03 0.518D-03

Coeff: -0.914D-03-0.291D-02-0.372D-03 0.866D-02 0.885D-02-0.247D-02

Coeff: -0.298D-01-0.748D-01-0.287D-02 0.248D+00 0.848D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=1.28D-08 MaxDP=6.89D-07 DE=-3.23D-11 OVMax= 9.93D-06

Cycle 18 Pass 1 IDiag 1:

RMSU= 2.41D-09 CP: 1.00D+00 1.39D+00 1.76D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.99D+00 1.56D+00 2.09D+00

CP: 1.74D+00 1.84D+00 1.39D+00 1.22D+00 1.30D+00

CP: 1.39D+00 1.30D+00

E= -1275.84200295306 Delta-E= -0.000000000026 Rises=F Damp=F

DIIS: error= 6.00D-08 at cycle 18 NSaved= 18.

NSaved=18 IEnMin=18 EnMin= -1275.84200295306 IErMin=18 ErrMin= 6.00D-08

ErrMax= 6.00D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.41D-12 BMatP= 4.47D-12

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

Coeff-Com: 0.892D-06-0.228D-04-0.222D-04-0.383D-04-0.152D-03 0.282D-03

Coeff-Com: 0.141D-03-0.404D-03-0.723D-03 0.361D-03 0.256D-02 0.482D-02

Coeff-Com: 0.178D-02-0.260D-01-0.114D+00-0.667D-01 0.552D+00 0.646D+00

Coeff: 0.892D-06-0.228D-04-0.222D-04-0.383D-04-0.152D-03 0.282D-03

Coeff: 0.141D-03-0.404D-03-0.723D-03 0.361D-03 0.256D-02 0.482D-02

Coeff: 0.178D-02-0.260D-01-0.114D+00-0.667D-01 0.552D+00 0.646D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=2.90D-09 MaxDP=1.86D-07 DE=-2.64D-11 OVMax= 1.36D-06

Error on total polarization charges = 0.06454

SCF Done: E(UB3LYP) = -1275.84200295 A.U. after 18 cycles

NFock= 18 Conv=0.29D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0179 S= 1.0060

<L.S>= 0.000000000000E+00

KE= 1.320738848404D+03 PE=-8.564184414146D+03 EE= 3.211456957111D+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 2.0179, after 2.0002

Leave Link 502 at Tue Sep 17 14:09:32 2019, MaxMem= 2415919104 cpu: 1713.3

(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= 15297 LenP2D= 41162.

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 = 247

Leave Link 701 at Tue Sep 17 14:09:36 2019, MaxMem= 2415919104 cpu: 68.1

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 14:09:36 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).

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 14:09:46 2019, MaxMem= 2415919104 cpu: 177.8

(Enter /home/blab/g09/l716.exe)

Dipole =-1.47437618D-13-8.34887715D-14-4.44089210D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000108760 0.001342476 -0.000000000

2 7 -0.000286389 0.004594124 -0.000000000

3 6 -0.001158341 0.004334875 0.000000000

4 6 0.000342914 -0.006886451 -0.000000000

5 6 0.001599995 0.001356918 0.000000000

6 7 0.004477703 0.002122736 0.000000000

7 6 -0.005726416 -0.001614671 0.000000000

8 7 -0.001187978 0.001205831 0.000000000

9 6 -0.003605501 0.006144959 -0.000000000

10 6 -0.001604712 -0.002876882 -0.000000000

11 6 0.001785657 -0.001084511 0.000000000

12 7 0.001956634 0.004221177 0.000000000

13 6 0.001604712 0.002876882 -0.000000000

14 6 -0.001785657 0.001084511 0.000000000

15 6 0.005726416 0.001614671 -0.000000000

16 7 0.001187978 -0.001205831 -0.000000000

17 6 0.003605501 -0.006144959 -0.000000000

18 7 -0.004477703 -0.002122736 0.000000000

19 7 0.000286389 -0.004594124 -0.000000000

20 6 0.001158341 -0.004334875 -0.000000000

21 6 -0.000342914 0.006886451 -0.000000000

22 6 -0.001599995 -0.001356918 0.000000000

23 6 -0.000108760 -0.001342476 -0.000000000

24 7 -0.001956634 -0.004221177 0.000000000

25 30 0.000000000 -0.000000000 0.000000000

26 6 -0.001704663 0.001878975 -0.000000000

27 1 -0.001204795 -0.000535682 -0.000000000

28 6 -0.000055802 0.000035254 0.000000000

29 1 -0.000713616 0.000305098 0.000000000

30 6 0.000055802 -0.000035254 -0.000000000

31 1 0.000713616 -0.000305098 0.000000000

32 6 0.001704663 -0.001878975 -0.000000000

33 1 0.001204795 0.000535682 0.000000000

34 1 -0.000372427 -0.000742455 0.000000000

35 1 0.000577536 0.000246166 0.001476776

36 1 0.000577536 0.000246166 -0.001476776

37 1 0.000634268 0.001101527 0.001780823

38 1 0.000634268 0.001101527 -0.001780823

39 1 0.001070162 -0.000403213 0.000000000

40 1 -0.000634268 -0.001101527 0.001780823

41 1 -0.000634268 -0.001101527 -0.001780823

42 1 -0.001070162 0.000403213 -0.000000000

43 1 -0.000577536 -0.000246166 0.001476776

44 1 -0.000577536 -0.000246166 -0.001476776

45 1 0.000372427 0.000742455 0.000000000

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

Cartesian Forces: Max 0.006886451 RMS 0.002003788

Leave Link 716 at Tue Sep 17 14:09:46 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 0.005303657 RMS 0.001129959

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= -2.70D-03 DEPred=-2.85D-03 R= 9.50D-01

TightC=F SS= 1.41D+00 RLast= 1.26D-01 DXNew= 2.1213D-01 3.7937D-01

Trust test= 9.50D-01 RLast= 1.26D-01 DXMaxT set to 2.12D-01

ITU= 1 -1 0 1 -1 1 1 1 1 0 0

Eigenvalues --- 0.00562 0.00878 0.00878 0.00878 0.00878

Eigenvalues --- 0.01336 0.01338 0.01339 0.01340 0.01605

Eigenvalues --- 0.01624 0.01633 0.01641 0.01773 0.01790

Eigenvalues --- 0.01807 0.01817 0.01889 0.01907 0.01940

Eigenvalues --- 0.01948 0.01998 0.01999 0.02045 0.02048

Eigenvalues --- 0.02070 0.02087 0.02101 0.02110 0.02113

Eigenvalues --- 0.02206 0.02314 0.02317 0.02352 0.02373

Eigenvalues --- 0.07214 0.07214 0.07236 0.07236 0.07259

Eigenvalues --- 0.07293 0.07392 0.07646 0.10732 0.13560

Eigenvalues --- 0.14493 0.14494 0.15636 0.15927 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16014

Eigenvalues --- 0.16149 0.16208 0.16298 0.17254 0.18547

Eigenvalues --- 0.21973 0.22073 0.22105 0.23841 0.23856

Eigenvalues --- 0.23988 0.24724 0.24997 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25024

Eigenvalues --- 0.25078 0.27424 0.30066 0.30286 0.32727

Eigenvalues --- 0.33199 0.33204 0.33282 0.33282 0.33387

Eigenvalues --- 0.33688 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33724 0.33866 0.34380 0.34434

Eigenvalues --- 0.34437 0.34437 0.35032 0.35538 0.35548

Eigenvalues --- 0.35557 0.35623 0.35682 0.35682 0.37243

Eigenvalues --- 0.38255 0.41577 0.41648 0.41825 0.42724

Eigenvalues --- 0.46443 0.48076 0.48972 0.49000 0.51355

Eigenvalues --- 0.51365 0.51686 0.53532 0.54017 0.54029

Eigenvalues --- 0.54958 0.56331 0.56334 0.56456

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 1.20334 -0.44320 0.05330 0.18656

Cosine: 0.980 > 0.710

Length: 0.915

GDIIS step was calculated using 4 of the last 11 vectors.

Iteration 1 RMS(Cart)= 0.01389466 RMS(Int)= 0.00003833

Iteration 2 RMS(Cart)= 0.00006885 RMS(Int)= 0.00000898

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000898

ITry= 1 IFail=0 DXMaxC= 5.89D-02 DCOld= 1.00D+10 DXMaxT= 2.12D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 5.36D-10 for atom 40.

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

(Linear) (Quad) (Total)

R1 2.58490 -0.00228 0.01246 -0.01473 -0.00228 2.58261

R2 2.73255 0.00089 -0.00573 0.00181 -0.00392 2.72863

R3 2.59478 -0.00255 -0.01329 0.00126 -0.01204 2.58273

R4 2.56386 -0.00048 -0.01143 0.01236 0.00091 2.56477

R5 3.81612 -0.00408 -0.01446 -0.00801 -0.02248 3.79364

R6 2.76435 0.00291 0.01257 -0.01040 0.00217 2.76652

R7 2.57743 0.00053 0.00448 -0.00349 0.00099 2.57843

R8 2.59764 0.00031 0.00350 0.00223 0.00574 2.60338

R9 2.82040 -0.00183 -0.00557 -0.00066 -0.00622 2.81417

R10 2.03931 0.00131 0.00346 0.00082 0.00427 2.04359

R11 2.50955 -0.00482 -0.00333 -0.00970 -0.01302 2.49653

R12 2.58238 -0.00068 -0.01057 0.01125 0.00070 2.58308

R13 2.79501 0.00108 0.00732 -0.00525 0.00207 2.79708

R14 2.58204 -0.00219 0.01026 -0.01173 -0.00146 2.58058

R15 3.80930 -0.00460 -0.02224 -0.01049 -0.03272 3.77658

R16 2.83411 0.00121 -0.00345 0.00162 -0.00183 2.83228

R17 2.49972 -0.00530 -0.01225 -0.00077 -0.01303 2.48670

R18 2.55260 -0.00004 0.00074 0.00155 0.00229 2.55489

R19 2.79964 0.00272 0.00858 0.00189 0.01047 2.81011

R20 2.04506 -0.00062 -0.00117 -0.00120 -0.00238 2.04268

R21 2.49972 -0.00530 -0.01225 -0.00077 -0.01303 2.48670

R22 2.55260 -0.00004 0.00074 0.00155 0.00229 2.55489

R23 2.83411 0.00121 -0.00345 0.00162 -0.00183 2.83228

R24 2.79964 0.00272 0.00858 0.00189 0.01047 2.81011

R25 2.79501 0.00108 0.00732 -0.00525 0.00207 2.79708

R26 2.04506 -0.00062 -0.00117 -0.00120 -0.00238 2.04268

R27 2.58238 -0.00068 -0.01057 0.01125 0.00070 2.58308

R28 2.50955 -0.00482 -0.00333 -0.00970 -0.01302 2.49653

R29 2.58204 -0.00219 0.01026 -0.01173 -0.00146 2.58058

R30 3.80930 -0.00460 -0.02224 -0.01049 -0.03272 3.77658

R31 2.57743 0.00053 0.00448 -0.00349 0.00099 2.57843

R32 2.56386 -0.00048 -0.01143 0.01236 0.00091 2.56477

R33 2.58490 -0.00228 0.01246 -0.01473 -0.00228 2.58261

R34 3.81612 -0.00408 -0.01446 -0.00801 -0.02248 3.79364

R35 2.76435 0.00291 0.01257 -0.01040 0.00217 2.76652

R36 2.59764 0.00031 0.00350 0.00223 0.00574 2.60338

R37 2.82040 -0.00183 -0.00557 -0.00066 -0.00622 2.81417

R38 2.73255 0.00089 -0.00573 0.00181 -0.00392 2.72863

R39 2.03931 0.00131 0.00346 0.00082 0.00427 2.04359

R40 2.59478 -0.00255 -0.01329 0.00126 -0.01204 2.58273

R41 2.06041 0.00075 0.00220 0.00029 0.00249 2.06290

R42 2.06522 0.00145 0.00491 0.00046 0.00537 2.07059

R43 2.06522 0.00145 0.00491 0.00046 0.00537 2.07059

R44 2.06267 0.00217 0.00590 0.00122 0.00712 2.06979

R45 2.06267 0.00217 0.00590 0.00122 0.00712 2.06979

R46 2.05863 0.00098 0.00294 0.00075 0.00369 2.06232

R47 2.06267 0.00217 0.00590 0.00122 0.00712 2.06979

R48 2.06267 0.00217 0.00590 0.00122 0.00712 2.06979

R49 2.05863 0.00098 0.00294 0.00075 0.00369 2.06232

R50 2.06522 0.00145 0.00491 0.00046 0.00537 2.07059

R51 2.06522 0.00145 0.00491 0.00046 0.00537 2.07059

R52 2.06041 0.00075 0.00220 0.00029 0.00249 2.06290

A1 1.88686 0.00095 0.00343 0.00515 0.00859 1.89546

A2 2.21148 -0.00117 -0.00902 0.00273 -0.00631 2.20517

A3 2.18484 0.00021 0.00559 -0.00789 -0.00228 2.18256

A4 1.91408 -0.00056 -0.00700 -0.00319 -0.01018 1.90390

A5 2.18681 0.00058 -0.00248 0.00418 0.00171 2.18852

A6 2.18229 -0.00002 0.00948 -0.00099 0.00848 2.19077

A7 1.88717 0.00132 0.00925 0.00049 0.00973 1.89690

A8 2.22352 -0.00017 -0.00050 -0.00505 -0.00555 2.21797

A9 2.17249 -0.00115 -0.00874 0.00455 -0.00418 2.16831

A10 1.86105 -0.00230 -0.00895 0.00105 -0.00790 1.85314

A11 2.17386 0.00083 0.00054 0.00426 0.00481 2.17867

A12 2.24827 0.00147 0.00841 -0.00531 0.00310 2.25137

A13 1.87561 0.00059 0.00328 -0.00351 -0.00024 1.87538

A14 2.18585 -0.00045 -0.00391 0.00281 -0.00110 2.18475

A15 2.22173 -0.00013 0.00063 0.00070 0.00134 2.22306

A16 2.17719 -0.00107 -0.01396 0.00558 -0.00835 2.16884

A17 2.22749 0.00100 0.00334 -0.00125 0.00212 2.22961

A18 2.17506 -0.00112 -0.00865 0.00352 -0.00514 2.16992

A19 1.88064 0.00012 0.00530 -0.00228 0.00303 1.88366

A20 1.91606 0.00071 -0.00389 -0.00019 -0.00408 1.91198

A21 2.18568 0.00015 0.00953 -0.00210 0.00742 2.19310

A22 2.18145 -0.00087 -0.00564 0.00229 -0.00334 2.17811

A23 1.88313 -0.00011 0.00157 0.00286 0.00444 1.88756

A24 2.24088 0.00129 -0.00227 0.00513 0.00287 2.24374

A25 2.15918 -0.00118 0.00070 -0.00799 -0.00730 2.15188

A26 1.85586 0.00013 0.00093 -0.00183 -0.00090 1.85497

A27 2.16890 -0.00190 -0.00776 -0.00076 -0.00852 2.16038

A28 2.25842 0.00178 0.00683 0.00260 0.00942 2.26784

A29 1.88909 -0.00085 -0.00392 0.00144 -0.00248 1.88661

A30 2.17085 -0.00005 -0.00329 -0.00059 -0.00389 2.16696

A31 2.22324 0.00090 0.00721 -0.00084 0.00637 2.22961

A32 2.17436 0.00026 0.01152 -0.01053 0.00096 2.17532

A33 1.85586 0.00013 0.00093 -0.00183 -0.00090 1.85497

A34 2.25842 0.00178 0.00683 0.00260 0.00942 2.26784

A35 2.16890 -0.00190 -0.00776 -0.00076 -0.00852 2.16038

A36 1.88909 -0.00085 -0.00392 0.00144 -0.00248 1.88661

A37 2.22324 0.00090 0.00721 -0.00084 0.00637 2.22961

A38 2.17085 -0.00005 -0.00329 -0.00059 -0.00389 2.16696

A39 1.88064 0.00012 0.00530 -0.00228 0.00303 1.88366

A40 2.17506 -0.00112 -0.00865 0.00352 -0.00514 2.16992

A41 2.22749 0.00100 0.00334 -0.00125 0.00212 2.22961

A42 1.91606 0.00071 -0.00389 -0.00019 -0.00408 1.91198

A43 2.18568 0.00015 0.00953 -0.00210 0.00742 2.19310

A44 2.18145 -0.00087 -0.00564 0.00229 -0.00334 2.17811

A45 2.15918 -0.00118 0.00070 -0.00799 -0.00730 2.15188

A46 2.24088 0.00129 -0.00227 0.00513 0.00287 2.24374

A47 1.88313 -0.00011 0.00157 0.00286 0.00444 1.88756

A48 2.17719 -0.00107 -0.01396 0.00558 -0.00835 2.16884

A49 1.91408 -0.00056 -0.00700 -0.00319 -0.01018 1.90390

A50 2.18229 -0.00002 0.00948 -0.00099 0.00848 2.19077

A51 2.18681 0.00058 -0.00248 0.00418 0.00171 2.18852

A52 2.22352 -0.00017 -0.00050 -0.00505 -0.00555 2.21797

A53 2.17249 -0.00115 -0.00874 0.00455 -0.00418 2.16831

A54 1.88717 0.00132 0.00925 0.00049 0.00973 1.89690

A55 1.86105 -0.00230 -0.00895 0.00105 -0.00790 1.85314

A56 2.17386 0.00083 0.00054 0.00426 0.00481 2.17867

A57 2.24827 0.00147 0.00841 -0.00531 0.00310 2.25137

A58 1.87561 0.00059 0.00328 -0.00351 -0.00024 1.87538

A59 2.22173 -0.00013 0.00063 0.00070 0.00134 2.22306

A60 2.18585 -0.00045 -0.00391 0.00281 -0.00110 2.18475

A61 1.88686 0.00095 0.00343 0.00515 0.00859 1.89546

A62 2.21148 -0.00117 -0.00902 0.00273 -0.00631 2.20517

A63 2.18484 0.00021 0.00559 -0.00789 -0.00228 2.18256

A64 2.17436 0.00026 0.01152 -0.01053 0.00096 2.17532

A65 1.57020 0.00010 -0.00788 0.00380 -0.00412 1.56609

A66 1.57139 -0.00010 0.00788 -0.00380 0.00412 1.57551

A67 1.57139 -0.00010 0.00788 -0.00380 0.00412 1.57551

A68 1.57020 0.00010 -0.00788 0.00380 -0.00412 1.56609

A69 1.93660 0.00082 0.00495 -0.00134 0.00362 1.94022

A70 1.94623 -0.00087 -0.00533 -0.00131 -0.00664 1.93958

A71 1.94623 -0.00087 -0.00533 -0.00131 -0.00664 1.93958

A72 1.88901 0.00008 0.00040 -0.00002 0.00039 1.88939

A73 1.88901 0.00008 0.00040 -0.00002 0.00039 1.88939

A74 1.85348 0.00080 0.00516 0.00427 0.00940 1.86288

A75 1.93460 0.00007 -0.00108 -0.00063 -0.00171 1.93289

A76 1.93460 0.00007 -0.00108 -0.00063 -0.00171 1.93289

A77 1.93882 0.00074 0.00302 0.00092 0.00395 1.94276

A78 1.85709 -0.00005 0.00437 0.00168 0.00605 1.86315

A79 1.89819 -0.00045 -0.00264 -0.00066 -0.00330 1.89489

A80 1.89819 -0.00045 -0.00264 -0.00066 -0.00330 1.89489

A81 1.93460 0.00007 -0.00108 -0.00063 -0.00171 1.93289

A82 1.93460 0.00007 -0.00108 -0.00063 -0.00171 1.93289

A83 1.93882 0.00074 0.00302 0.00092 0.00395 1.94276

A84 1.85709 -0.00005 0.00437 0.00168 0.00605 1.86315

A85 1.89819 -0.00045 -0.00264 -0.00066 -0.00330 1.89489

A86 1.89819 -0.00045 -0.00264 -0.00066 -0.00330 1.89489

A87 1.94623 -0.00087 -0.00533 -0.00131 -0.00664 1.93958

A88 1.94623 -0.00087 -0.00533 -0.00131 -0.00664 1.93958

A89 1.93660 0.00082 0.00495 -0.00134 0.00362 1.94022

A90 1.85348 0.00080 0.00516 0.00427 0.00940 1.86288

A91 1.88901 0.00008 0.00040 -0.00002 0.00039 1.88939

A92 1.88901 0.00008 0.00040 -0.00002 0.00039 1.88939

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 1.03436 -0.00007 -0.00030 0.00183 0.00155 1.03591

D31 -1.03436 0.00007 0.00030 -0.00183 -0.00155 -1.03591

D32 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.10724 -0.00007 -0.00030 0.00183 0.00155 -2.10569

D34 2.10724 0.00007 0.00030 -0.00183 -0.00155 2.10569

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

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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 1.02909 0.00001 0.00203 0.00065 0.00268 1.03177

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D66 -2.11250 0.00001 0.00203 0.00065 0.00268 -2.10983

D67 2.11250 -0.00001 -0.00203 -0.00065 -0.00268 2.10983

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D71 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

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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 -2.11250 0.00001 0.00203 0.00065 0.00268 -2.10983

D80 2.11250 -0.00001 -0.00203 -0.00065 -0.00268 2.10983

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D83 -1.02909 -0.00001 -0.00203 -0.00065 -0.00268 -1.03177

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

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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

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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

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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

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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 1.03436 -0.00007 -0.00030 0.00183 0.00155 1.03591

D126 -1.03436 0.00007 0.00030 -0.00183 -0.00155 -1.03591

D127 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D128 -2.10724 -0.00007 -0.00030 0.00183 0.00155 -2.10569

D129 2.10724 0.00007 0.00030 -0.00183 -0.00155 2.10569

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 0.005304 0.000450 NO

RMS Force 0.001130 0.000300 NO

Maximum Displacement 0.058936 0.001800 NO

RMS Displacement 0.013931 0.001200 NO

Predicted change in Energy=-7.255219D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:09:46 2019, MaxMem= 2415919104 cpu: 1.4

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.067208 -2.191474 0.000000

2 7 0 -0.739816 -1.866216 0.000000

3 6 0 -0.003530 -3.006359 0.000000

4 6 0 -0.914117 -4.152685 0.000000

5 6 0 -2.188874 -3.630270 0.000000

6 7 0 1.357203 -3.106924 0.000000

7 6 0 2.179473 -2.072905 0.000000

8 7 0 1.854332 -0.745233 0.000000

9 6 0 2.995580 0.004680 0.000000

10 6 0 4.167858 -0.929184 0.000000

11 6 0 3.655712 -2.180414 0.000000

12 7 0 -3.115944 -1.315067 0.000000

13 6 0 -4.167858 0.929184 0.000000

14 6 0 -3.655712 2.180414 0.000000

15 6 0 -2.179473 2.072905 0.000000

16 7 0 -1.854332 0.745233 0.000000

17 6 0 -2.995580 -0.004680 0.000000

18 7 0 -1.357203 3.106924 0.000000

19 7 0 0.739816 1.866216 0.000000

20 6 0 0.003530 3.006359 0.000000

21 6 0 0.914117 4.152685 0.000000

22 6 0 2.188874 3.630270 0.000000

23 6 0 2.067208 2.191474 0.000000

24 7 0 3.115944 1.315067 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.485944 -5.579000 0.000000

27 1 0 -3.122155 -4.176581 0.000000

28 6 0 5.584683 -0.477623 0.000000

29 1 0 4.196061 -3.116606 0.000000

30 6 0 -5.584683 0.477623 0.000000

31 1 0 -4.196061 3.116606 0.000000

32 6 0 0.485944 5.579000 0.000000

33 1 0 3.122155 4.176581 0.000000

34 1 0 -1.347619 -6.249218 0.000000

35 1 0 0.126604 -5.807514 0.879284

36 1 0 0.126604 -5.807514 -0.879284

37 1 0 5.794690 0.141124 0.879031

38 1 0 5.794690 0.141124 -0.879031

39 1 0 6.271329 -1.325868 0.000000

40 1 0 -5.794690 -0.141124 0.879031

41 1 0 -5.794690 -0.141124 -0.879031

42 1 0 -6.271329 1.325868 0.000000

43 1 0 -0.126604 5.807514 0.879284

44 1 0 -0.126604 5.807514 -0.879284

45 1 0 1.347619 6.249218 0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.366661 0.000000

3 C 2.218739 1.357219 0.000000

4 C 2.275076 2.293102 1.463977 0.000000

5 C 1.443931 2.282904 2.272661 1.377651 0.000000

6 N 3.544663 2.436564 1.364444 2.500501 3.584487

7 C 4.248336 2.926597 2.374203 3.727704 4.637654

8 N 4.179724 2.825989 2.926491 4.390335 4.966986

9 C 5.518597 4.177731 4.249826 5.706961 6.331778

10 C 6.361558 4.996328 4.659950 6.018091 6.906801

11 C 5.722931 4.406743 3.751298 4.977267 6.021732

12 N 1.366724 2.439210 3.542257 3.591673 2.493917

13 C 3.761812 4.423317 5.729758 6.034254 4.970412

14 C 4.651532 4.987751 6.343583 6.901050 5.992967

15 C 4.265856 4.193958 5.525726 6.352880 5.703182

16 N 2.944412 2.839333 4.183289 4.987344 4.388273

17 C 2.375697 2.924685 4.238211 4.640951 3.714253

18 N 5.345758 5.011316 6.261363 7.273118 6.788332

19 N 4.933987 4.015017 4.928951 6.242008 6.228048

20 C 5.595125 4.928951 6.012722 7.217616 6.989383

21 C 7.009753 6.242008 7.217616 8.504211 8.378719

22 C 7.211583 6.228048 6.989383 8.378719 8.478213

23 C 6.025249 4.933987 5.595125 7.009753 7.211583

24 N 6.257866 4.998745 5.329713 6.792474 7.252409

25 Zn 3.012624 2.007509 3.006361 4.252105 4.239107

26 C 3.738413 3.721453 2.617480 1.489197 2.587957

27 H 2.248013 3.318632 3.330951 2.208167 1.081420

28 C 7.841474 6.475143 6.133729 7.465954 8.388526

29 H 6.331225 5.091794 4.201039 5.214152 6.405564

30 C 4.415507 5.382036 6.579315 6.576772 5.329756

31 H 5.719066 6.064169 7.420782 7.975822 7.039114

32 C 8.179171 7.545445 8.599301 9.831880 9.589854

33 H 8.214719 7.171486 7.833552 9.255709 9.442136

34 H 4.121056 4.424944 3.510372 2.140882 2.750746

35 H 4.319919 4.130092 2.938800 2.143525 3.297722

36 H 4.319919 4.130092 2.938800 2.143525 3.297722

37 H 8.247615 6.892161 6.655728 8.013587 8.873184

38 H 8.247615 6.892161 6.655728 8.013587 8.873184

39 H 8.383345 7.031937 6.495992 7.721497 8.768426

40 H 4.344048 5.412983 6.520721 6.378504 5.093991

41 H 4.344048 5.412983 6.520721 6.378504 5.093991

42 H 5.481453 6.386473 7.619284 7.662523 6.421039

43 H 8.277856 7.748246 8.858479 10.029899 9.700405

44 H 8.277856 7.748246 8.858479 10.029899 9.700405

45 H 9.105291 8.379598 9.353679 10.644953 10.493382

6 7 8 9 10

6 N 0.000000

7 C 1.321107 0.000000

8 N 2.413447 1.366905 0.000000

9 C 3.516584 2.232127 1.365582 0.000000

10 C 3.555606 2.293855 2.320827 1.498779 0.000000

11 C 2.478218 1.480149 2.303196 2.282633 1.351987

12 N 4.818691 5.349369 5.002835 6.252395 7.294016

13 C 6.842256 7.021477 6.250636 7.222848 8.540356

14 C 7.285963 7.220810 6.238589 6.998106 8.418898

15 C 6.272057 6.015658 4.920720 5.573035 7.021477

16 N 5.015284 4.920720 3.996959 4.906125 6.250636

17 C 5.345150 5.573035 4.906125 5.991166 7.222848

18 N 6.780848 6.272057 5.015284 5.345150 6.842256

19 N 5.011316 4.193958 2.839333 2.924685 4.423317

20 C 6.261363 5.525726 4.183289 4.238211 5.729758

21 C 7.273118 6.352880 4.987344 4.640951 6.034254

22 C 6.788332 5.703182 4.388273 3.714253 4.970412

23 C 5.345758 4.265856 2.944412 2.375697 3.761812

24 N 4.758905 3.515015 2.415885 1.315903 2.478546

25 Zn 3.390424 3.007829 1.998480 2.995583 4.270178

26 C 3.083561 4.404220 5.370493 6.580159 6.578651

27 H 4.605302 5.703745 6.044797 7.410102 7.980593

28 C 4.978435 3.760370 3.739937 2.633642 1.487044

29 H 2.838875 2.270670 3.332732 3.344186 2.187603

30 C 7.812730 8.172350 7.538854 8.593287 9.853484

31 H 8.340927 8.220611 7.177817 7.836056 9.291047

32 C 8.729511 7.837071 6.470580 6.113208 7.477496

33 H 7.494298 6.320183 5.082482 4.173820 5.211749

34 H 4.146091 5.466440 6.367602 7.614107 7.663109

35 H 3.095271 4.351404 5.420782 6.541083 6.395543

36 H 3.095271 4.351404 5.420782 6.541083 6.395543

37 H 5.569004 4.329482 4.133369 2.937062 2.136549

38 H 5.569004 4.329482 4.133369 2.937062 2.136549

39 H 5.226930 4.159489 4.454997 3.535660 2.140549

40 H 7.792191 8.251772 7.723030 8.835315 10.032253

41 H 7.792191 8.251772 7.723030 8.835315 10.032253

42 H 8.822933 9.108661 8.385454 9.360616 10.679976

43 H 9.079760 8.257853 6.901865 6.647861 8.037329

44 H 9.079760 8.257853 6.901865 6.647861 8.037329

45 H 9.356147 8.363594 7.012781 6.458330 7.712536

11 12 13 14 15

11 C 0.000000

12 N 6.826723 0.000000

13 C 8.418898 2.478546 0.000000

14 C 8.513151 3.536911 1.351987 0.000000

15 C 7.220810 3.515015 2.293855 1.480149 0.000000

16 N 6.238589 2.415885 2.320827 2.303196 1.366905

17 C 6.998106 1.315903 1.498779 2.282633 2.232127

18 N 7.285963 4.758905 3.555606 2.478218 1.321107

19 N 4.987751 4.998745 4.996328 4.406743 2.926597

20 C 6.343583 5.329713 4.659950 3.751298 2.374203

21 C 6.901050 6.792474 6.018091 4.977267 3.727704

22 C 5.992967 7.252409 6.906801 6.021732 4.637654

23 C 4.651532 6.257866 6.361558 5.722931 4.248336

24 N 3.536911 6.764172 7.294016 6.826723 5.349369

25 Zn 4.256575 3.382086 4.270178 4.256575 3.007829

26 C 5.357583 5.009793 7.477496 8.381882 7.837071

27 H 7.065703 2.861520 5.211749 6.379347 6.320183

28 C 2.573019 8.740836 9.853484 9.615095 8.172350

29 H 1.080940 7.530668 9.291047 9.471471 8.220611

30 C 9.615095 3.050969 1.487044 2.573019 3.760370

31 H 9.471471 4.561401 2.187603 1.080940 2.270670

32 C 8.381882 7.778288 6.578651 5.357583 4.404220

33 H 6.379347 8.310961 7.980593 7.065703 5.703745

34 H 6.448914 5.241452 7.712536 8.739908 8.363594

35 H 5.136497 5.609754 8.037329 8.881782 8.257853

36 H 5.136497 5.609754 8.037329 8.881782 8.257853

37 H 3.276807 9.071526 10.032253 9.707806 8.251772

38 H 3.276807 9.071526 10.032253 9.707806 8.251772

39 H 2.751673 9.387279 10.679976 10.528065 9.108661

40 H 9.707806 3.053935 2.136549 3.276807 4.329482

41 H 9.707806 3.053935 2.136549 3.276807 4.329482

42 H 10.528065 4.114729 2.140549 2.751673 4.159489

43 H 8.881782 7.774346 6.395543 5.136497 4.351404

44 H 8.881782 7.774346 6.395543 5.136497 4.351404

45 H 8.739908 8.783041 7.663109 6.448914 5.466440

16 17 18 19 20

16 N 0.000000

17 C 1.365582 0.000000

18 N 2.413447 3.516584 0.000000

19 N 2.825989 4.177731 2.436564 0.000000

20 C 2.926491 4.249826 1.364444 1.357219 0.000000

21 C 4.390335 5.706961 2.500501 2.293102 1.463977

22 C 4.966986 6.331778 3.584487 2.282904 2.272661

23 C 4.179724 5.518597 3.544663 1.366661 2.218739

24 N 5.002835 6.252395 4.818691 2.439210 3.542257

25 Zn 1.998480 2.995583 3.390424 2.007509 3.006361

26 C 6.470580 6.113208 8.729511 7.545445 8.599301

27 H 5.082482 4.173820 7.494298 7.171486 7.833552

28 C 7.538854 8.593287 7.812730 5.382036 6.579315

29 H 7.177817 7.836056 8.340927 6.064169 7.420782

30 C 3.739937 2.633642 4.978435 6.475143 6.133729

31 H 3.332732 3.344186 2.838875 5.091794 4.201039

32 C 5.370493 6.580159 3.083561 3.721453 2.617480

33 H 6.044797 7.410102 4.605302 3.318632 3.330951

34 H 7.012781 6.458330 9.356147 8.379598 9.353679

35 H 6.901865 6.647861 9.079760 7.748246 8.858479

36 H 6.901865 6.647861 9.079760 7.748246 8.858479

37 H 7.723030 8.835315 7.792191 5.412983 6.520721

38 H 7.723030 8.835315 7.792191 5.412983 6.520721

39 H 8.385454 9.360616 8.822933 6.386473 7.619284

40 H 4.133369 2.937062 5.569004 6.892161 6.655728

41 H 4.133369 2.937062 5.569004 6.892161 6.655728

42 H 4.454997 3.535660 5.226930 7.031937 6.495992

43 H 5.420782 6.541083 3.095271 4.130092 2.938800

44 H 5.420782 6.541083 3.095271 4.130092 2.938800

45 H 6.367602 7.614107 4.146091 4.424944 3.510372

21 22 23 24 25

21 C 0.000000

22 C 1.377651 0.000000

23 C 2.275076 1.443931 0.000000

24 N 3.591673 2.493917 1.366724 0.000000

25 Zn 4.252105 4.239107 3.012624 3.382086 0.000000

26 C 9.831880 9.589854 8.179171 7.778288 5.600124

27 H 9.255709 9.442136 8.214719 8.310961 5.214564

28 C 6.576772 5.329756 4.415507 3.050969 5.605070

29 H 7.975822 7.039114 5.719066 4.561401 5.226869

30 C 7.465954 8.388526 7.841474 8.740836 5.605070

31 H 5.214152 6.405564 6.331225 7.530668 5.226869

32 C 1.489197 2.587957 3.738413 5.009793 5.600124

33 H 2.208167 1.081420 2.248013 2.861520 5.214564

34 H 10.644953 10.493382 9.105291 8.783041 6.392872

35 H 10.029899 9.700405 8.277856 7.774346 5.875065

36 H 10.029899 9.700405 8.277856 7.774346 5.875065

37 H 6.378504 5.093991 4.344048 3.053935 5.862682

38 H 6.378504 5.093991 4.344048 3.053935 5.862682

39 H 7.662523 6.421039 5.481453 4.114729 6.409953

40 H 8.013587 8.873184 8.247615 9.071526 5.862682

41 H 8.013587 8.873184 8.247615 9.071526 5.862682

42 H 7.721497 8.768426 8.383345 9.387279 6.409953

43 H 2.143525 3.297722 4.319919 5.609754 5.875065

44 H 2.143525 3.297722 4.319919 5.609754 5.875065

45 H 2.140882 2.750746 4.121056 5.241452 6.392872

26 27 28 29 30

26 C 0.000000

27 H 2.986032 0.000000

28 C 7.929474 9.459985 0.000000

29 H 5.290043 7.394581 2.982030 0.000000

30 C 7.917059 5.265516 11.210139 10.420241 0.000000

31 H 9.454022 7.371828 10.420241 10.453738 2.982030

32 C 11.200247 10.401429 7.917059 9.454022 7.929474

33 H 10.401429 10.429128 5.265516 7.371828 9.459985

34 H 1.091639 2.728517 9.020428 6.367547 7.950038

35 H 1.095707 3.739989 7.679291 4.957279 8.537850

36 H 1.095707 3.739989 7.679291 4.957279 8.537850

37 H 8.540426 9.946125 1.095284 3.733780 11.418233

38 H 8.540426 9.946125 1.095284 3.733780 11.418233

39 H 7.984351 9.816522 1.091331 2.741072 11.992397

40 H 7.650227 4.919355 11.418233 10.461420 1.095284

41 H 7.650227 4.919355 11.418233 10.461420 1.095284

42 H 9.008212 6.339893 11.992397 11.371096 1.091331

43 H 11.426066 10.460813 8.537850 9.954823 7.679291

44 H 11.426066 10.460813 8.537850 9.954823 7.679291

45 H 11.969490 11.343552 7.950038 9.789396 9.020428

31 32 33 34 35

31 H 0.000000

32 C 5.290043 0.000000

33 H 7.394581 2.986032 0.000000

34 H 9.789396 11.969490 11.343552 0.000000

35 H 9.954823 11.426066 10.460813 1.772449 0.000000

36 H 9.954823 11.426066 10.460813 1.772449 1.758567

37 H 10.461420 7.650227 4.919355 9.624020 8.216660

38 H 10.461420 7.650227 4.919355 9.624020 8.402688

39 H 11.371096 9.008212 6.339893 9.071259 7.656105

40 H 3.733780 8.540426 9.946125 7.606441 8.195713

41 H 3.733780 8.540426 9.946125 7.606441 8.382206

42 H 2.741072 7.984351 9.816522 9.034647 9.622465

43 H 4.957279 1.095707 3.739989 12.150260 11.617788

44 H 4.957279 1.095707 3.739989 12.150260 11.750131

45 H 6.367547 1.091639 2.728517 12.785743 12.150260

36 37 38 39 40

36 H 0.000000

37 H 8.402688 0.000000

38 H 8.216660 1.758062 0.000000

39 H 7.656105 1.775372 1.775372 0.000000

40 H 8.382206 11.592817 11.725365 12.155868 0.000000

41 H 8.195713 11.725365 11.592817 12.155868 1.758062

42 H 9.622465 12.155868 12.155868 12.819905 1.775372

43 H 11.750131 8.195713 8.382206 9.622465 8.216660

44 H 11.617788 8.382206 8.195713 9.622465 8.402688

45 H 12.150260 7.606441 7.606441 9.034647 9.624020

41 42 43 44 45

41 H 0.000000

42 H 1.775372 0.000000

43 H 8.402688 7.656105 0.000000

44 H 8.216660 7.656105 1.758567 0.000000

45 H 9.624020 9.071259 1.772449 1.772449 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=0 Diff= 5.71D-03

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 2.804268 -1.100904 0.000000

2 7 0 2.007486 0.009457 0.000000

3 6 0 2.790832 1.117795 0.000000

4 6 0 4.194032 0.700352 0.000000

5 6 0 4.184655 -0.677267 0.000000

6 7 0 2.376726 2.417881 0.000000

7 6 0 1.110664 2.795257 0.000000

8 7 0 0.000000 1.998480 0.000000

9 6 0 -1.121394 2.777768 0.000000

10 6 0 -0.692030 4.213729 0.000000

11 6 0 0.659930 4.205107 0.000000

12 7 0 2.382148 -2.400807 0.000000

13 6 0 0.692030 -4.213729 0.000000

14 6 0 -0.659930 -4.205107 0.000000

15 6 0 -1.110664 -2.795257 0.000000

16 7 0 -0.000000 -1.998480 0.000000

17 6 0 1.121394 -2.777768 0.000000

18 7 0 -2.376726 -2.417881 0.000000

19 7 0 -2.007486 -0.009457 0.000000

20 6 0 -2.790832 -1.117795 0.000000

21 6 0 -4.194032 -0.700352 0.000000

22 6 0 -4.184655 0.677267 0.000000

23 6 0 -2.804268 1.100904 0.000000

24 7 0 -2.382148 2.400807 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 5.357804 1.629515 0.000000

27 1 0 5.039582 -1.339513 0.000000

28 6 0 -1.639355 5.359974 0.000000

29 1 0 1.327099 5.055588 0.000000

30 6 0 1.639355 -5.359974 0.000000

31 1 0 -1.327099 -5.055588 0.000000

32 6 0 -5.357804 -1.629515 0.000000

33 1 0 -5.039582 1.339513 0.000000

34 1 0 6.300999 1.079915 0.000000

35 1 0 5.341417 2.283093 0.879284

36 1 0 5.341417 2.283093 -0.879284

37 1 0 -2.291784 5.324103 0.879031

38 1 0 -2.291784 5.324103 -0.879031

39 1 0 -1.108342 6.313404 0.000000

40 1 0 2.291784 -5.324103 0.879031

41 1 0 2.291784 -5.324103 -0.879031

42 1 0 1.108342 -6.313404 0.000000

43 1 0 -5.341417 -2.283093 0.879284

44 1 0 -5.341417 -2.283093 -0.879284

45 1 0 -6.300999 -1.079915 0.000000

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

Rotational constants (GHZ): 0.1829191 0.1821355 0.0914691

Leave Link 202 at Tue Sep 17 14:09:46 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 101 beta electrons

nuclear repulsion energy 2762.5345051772 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= -0.1142244178 Hartrees.

Nuclear repulsion after empirical dispersion term = 2762.4202807593 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 = 3498

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.13D-08

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 132

GePol: Fraction of low-weight points (<1% of avg) = 3.77%

GePol: Cavity surface area = 381.868 Ang\*\*2

GePol: Cavity volume = 379.111 Ang\*\*3

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

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

PCM non-electrostatic energy = -0.0106807470 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2762.4096000123 Hartrees.

Leave Link 301 at Tue Sep 17 14:09:46 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= 15329 LenP2D= 41268.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.83D-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 14:09:47 2019, MaxMem= 2415919104 cpu: 12.9

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:09:47 2019, MaxMem= 2415919104 cpu: 1.4

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999998 -0.000000 0.000000 -0.001793 Ang= -0.21 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 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0179 S= 1.0059

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= -1276.14806979375

Leave Link 401 at Tue Sep 17 14:09:49 2019, MaxMem= 2415919104 cpu: 40.3

(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= 36708012.

Iteration 1 A\*A^-1 deviation from unit magnitude is 1.05D-14 for 3498.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.95D-15 for 3498 2628.

Iteration 1 A^-1\*A deviation from unit magnitude is 1.05D-14 for 3498.

Iteration 1 A^-1\*A deviation from orthogonality is 5.51D-11 for 2441 2385.

E= -1275.84197483796

DIIS: error= 1.58D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.84197483796 IErMin= 1 ErrMin= 1.58D-03

ErrMax= 1.58D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.56D-03 BMatP= 2.56D-03

IDIUse=3 WtCom= 9.84D-01 WtEn= 1.58D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.304 Goal= None Shift= 0.000

Gap= 0.393 Goal= None Shift= 0.000

GapD= 0.304 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.

RMSDP=6.50D-05 MaxDP=1.75D-03 OVMax= 3.96D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 6.50D-05 CP: 1.00D+00

E= -1275.84246238338 Delta-E= -0.000487545422 Rises=F Damp=F

DIIS: error= 5.95D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84246238338 IErMin= 2 ErrMin= 5.95D-04

ErrMax= 5.95D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.16D-04 BMatP= 2.56D-03

IDIUse=3 WtCom= 9.94D-01 WtEn= 5.95D-03

Coeff-Com: 0.144D+00 0.856D+00

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

Coeff: 0.143D+00 0.857D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=2.88D-05 MaxDP=1.33D-03 DE=-4.88D-04 OVMax= 4.47D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.86D-05 CP: 1.00D+00 9.51D-01

E= -1275.84242997922 Delta-E= 0.000032404162 Rises=F Damp=F

DIIS: error= 6.18D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1275.84246238338 IErMin= 2 ErrMin= 5.95D-04

ErrMax= 6.18D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.64D-04 BMatP= 3.16D-04

IDIUse=3 WtCom= 2.87D-01 WtEn= 7.13D-01

Coeff-Com: -0.806D-02 0.552D+00 0.456D+00

Coeff-En: 0.000D+00 0.580D+00 0.420D+00

Coeff: -0.231D-02 0.572D+00 0.430D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=1.58D-05 MaxDP=6.43D-04 DE= 3.24D-05 OVMax= 2.58D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 5.18D-06 CP: 1.00D+00 1.00D+00 4.91D-01

E= -1275.84253096609 Delta-E= -0.000100986872 Rises=F Damp=F

DIIS: error= 1.06D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84253096609 IErMin= 4 ErrMin= 1.06D-04

ErrMax= 1.06D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.36D-06 BMatP= 3.16D-04

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.06D-03

Coeff-Com: -0.903D-02 0.273D+00 0.219D+00 0.517D+00

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

Coeff: -0.902D-02 0.273D+00 0.219D+00 0.518D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=2.84D-06 MaxDP=1.40D-04 DE=-1.01D-04 OVMax= 6.98D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.07D-06 CP: 1.00D+00 1.01D+00 4.87D-01 6.37D-01

E= -1275.84253274333 Delta-E= -0.000001777234 Rises=F Damp=F

DIIS: error= 4.11D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84253274333 IErMin= 5 ErrMin= 4.11D-05

ErrMax= 4.11D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.31D-06 BMatP= 9.36D-06

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

Coeff-Com: -0.352D-02 0.694D-01 0.551D-01 0.284D+00 0.595D+00

Coeff: -0.352D-02 0.694D-01 0.551D-01 0.284D+00 0.595D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=1.15D-06 MaxDP=6.10D-05 DE=-1.78D-06 OVMax= 3.33D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 7.94D-07 CP: 1.00D+00 1.01D+00 4.84D-01 7.64D-01 7.60D-01

E= -1275.84253302278 Delta-E= -0.000000279454 Rises=F Damp=F

DIIS: error= 1.54D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84253302278 IErMin= 6 ErrMin= 1.54D-05

ErrMax= 1.54D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.95D-07 BMatP= 1.31D-06

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

Coeff-Com: -0.992D-03 0.109D-01 0.887D-02 0.108D+00 0.340D+00 0.533D+00

Coeff: -0.992D-03 0.109D-01 0.887D-02 0.108D+00 0.340D+00 0.533D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=4.41D-07 MaxDP=2.00D-05 DE=-2.79D-07 OVMax= 1.37D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 3.15D-07 CP: 1.00D+00 1.01D+00 4.87D-01 7.58D-01 8.92D-01

CP: 8.65D-01

E= -1275.84253308042 Delta-E= -0.000000057637 Rises=F Damp=F

DIIS: error= 7.20D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84253308042 IErMin= 7 ErrMin= 7.20D-06

ErrMax= 7.20D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.16D-08 BMatP= 1.95D-07

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

Coeff-Com: 0.259D-03-0.106D-01-0.820D-02-0.999D-02 0.305D-01 0.243D+00

Coeff-Com: 0.755D+00

Coeff: 0.259D-03-0.106D-01-0.820D-02-0.999D-02 0.305D-01 0.243D+00

Coeff: 0.755D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=2.59D-07 MaxDP=1.28D-05 DE=-5.76D-08 OVMax= 1.50D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.76D-07 CP: 1.00D+00 1.01D+00 4.88D-01 7.78D-01 9.31D-01

CP: 1.03D+00 1.07D+00

E= -1275.84253309508 Delta-E= -0.000000014667 Rises=F Damp=F

DIIS: error= 2.96D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84253309508 IErMin= 8 ErrMin= 2.96D-06

ErrMax= 2.96D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.60D-09 BMatP= 2.16D-08

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

Coeff-Com: 0.302D-03-0.691D-02-0.553D-02-0.215D-01-0.430D-01 0.271D-01

Coeff-Com: 0.358D+00 0.692D+00

Coeff: 0.302D-03-0.691D-02-0.553D-02-0.215D-01-0.430D-01 0.271D-01

Coeff: 0.358D+00 0.692D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=1.41D-07 MaxDP=7.12D-06 DE=-1.47D-08 OVMax= 7.52D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 7.02D-08 CP: 1.00D+00 1.01D+00 4.88D-01 7.80D-01 9.59D-01

CP: 1.10D+00 1.34D+00 1.17D+00

E= -1275.84253309963 Delta-E= -0.000000004550 Rises=F Damp=F

DIIS: error= 1.90D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84253309963 IErMin= 9 ErrMin= 1.90D-06

ErrMax= 1.90D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.17D-09 BMatP= 5.60D-09

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

Coeff-Com: 0.211D-04 0.182D-02 0.118D-02-0.636D-02-0.436D-01-0.106D+00

Coeff-Com: -0.162D+00 0.422D+00 0.894D+00

Coeff: 0.211D-04 0.182D-02 0.118D-02-0.636D-02-0.436D-01-0.106D+00

Coeff: -0.162D+00 0.422D+00 0.894D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=1.34D-07 MaxDP=7.55D-06 DE=-4.55D-09 OVMax= 7.07D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 5.14D-08 CP: 1.00D+00 1.01D+00 4.88D-01 7.85D-01 9.84D-01

CP: 1.17D+00 1.51D+00 1.59D+00 1.21D+00

E= -1275.84253310206 Delta-E= -0.000000002432 Rises=F Damp=F

DIIS: error= 9.41D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84253310206 IErMin=10 ErrMin= 9.41D-07

ErrMax= 9.41D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.98D-10 BMatP= 2.17D-09

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

Coeff-Com: -0.211D-04 0.177D-02 0.120D-02 0.119D-03-0.157D-01-0.540D-01

Coeff-Com: -0.135D+00 0.105D+00 0.454D+00 0.642D+00

Coeff: -0.211D-04 0.177D-02 0.120D-02 0.119D-03-0.157D-01-0.540D-01

Coeff: -0.135D+00 0.105D+00 0.454D+00 0.642D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=4.46D-08 MaxDP=2.70D-06 DE=-2.43D-09 OVMax= 2.14D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 2.55D-08 CP: 1.00D+00 1.01D+00 4.88D-01 7.86D-01 9.87D-01

CP: 1.18D+00 1.57D+00 1.69D+00 1.46D+00 1.27D+00

E= -1275.84253310245 Delta-E= -0.000000000382 Rises=F Damp=F

DIIS: error= 4.61D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84253310245 IErMin=11 ErrMin= 4.61D-07

ErrMax= 4.61D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.65D-10 BMatP= 4.98D-10

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

Coeff-Com: -0.284D-04 0.339D-03 0.197D-03 0.321D-02 0.879D-02 0.171D-01

Coeff-Com: -0.714D-02-0.113D+00-0.125D+00 0.313D+00 0.902D+00

Coeff: -0.284D-04 0.339D-03 0.197D-03 0.321D-02 0.879D-02 0.171D-01

Coeff: -0.714D-02-0.113D+00-0.125D+00 0.313D+00 0.902D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=4.25D-08 MaxDP=2.77D-06 DE=-3.82D-10 OVMax= 2.50D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.40D-08 CP: 1.00D+00 1.01D+00 4.89D-01 7.85D-01 9.92D-01

CP: 1.19D+00 1.59D+00 1.77D+00 1.71D+00 1.79D+00

CP: 1.64D+00

E= -1275.84253310270 Delta-E= -0.000000000249 Rises=F Damp=F

DIIS: error= 3.28D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84253310270 IErMin=12 ErrMin= 3.28D-07

ErrMax= 3.28D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.68D-11 BMatP= 1.65D-10

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

Coeff-Com: -0.588D-05-0.410D-03-0.338D-03 0.189D-02 0.853D-02 0.278D-01

Coeff-Com: 0.383D-01-0.889D-01-0.211D+00-0.217D-01 0.370D+00 0.876D+00

Coeff: -0.588D-05-0.410D-03-0.338D-03 0.189D-02 0.853D-02 0.278D-01

Coeff: 0.383D-01-0.889D-01-0.211D+00-0.217D-01 0.370D+00 0.876D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=3.34D-08 MaxDP=1.83D-06 DE=-2.49D-10 OVMax= 2.22D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 9.16D-09 CP: 1.00D+00 1.01D+00 4.88D-01 7.85D-01 9.94D-01

CP: 1.19D+00 1.60D+00 1.80D+00 1.86D+00 2.20D+00

CP: 2.39D+00 1.48D+00

E= -1275.84253310280 Delta-E= -0.000000000104 Rises=F Damp=F

DIIS: error= 2.32D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84253310280 IErMin=13 ErrMin= 2.32D-07

ErrMax= 2.32D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.78D-11 BMatP= 5.68D-11

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

Coeff-Com: 0.717D-05-0.461D-03-0.365D-03 0.112D-03 0.163D-02 0.137D-01

Coeff-Com: 0.302D-01-0.168D-01-0.104D+00-0.113D+00-0.154D+00 0.626D+00

Coeff-Com: 0.716D+00

Coeff: 0.717D-05-0.461D-03-0.365D-03 0.112D-03 0.163D-02 0.137D-01

Coeff: 0.302D-01-0.168D-01-0.104D+00-0.113D+00-0.154D+00 0.626D+00

Coeff: 0.716D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=2.50D-08 MaxDP=1.23D-06 DE=-1.04D-10 OVMax= 1.77D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 5.23D-09 CP: 1.00D+00 1.01D+00 4.89D-01 7.85D-01 9.95D-01

CP: 1.19D+00 1.61D+00 1.83D+00 1.98D+00 2.48D+00

CP: 2.90D+00 2.18D+00 1.43D+00

E= -1275.84253310284 Delta-E= -0.000000000040 Rises=F Damp=F

DIIS: error= 1.70D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84253310284 IErMin=14 ErrMin= 1.70D-07

ErrMax= 1.70D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.60D-12 BMatP= 3.78D-11

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

Coeff-Com: 0.469D-05-0.102D-03-0.904D-04-0.208D-03-0.143D-02 0.101D-02

Coeff-Com: 0.429D-02 0.121D-01-0.265D-02-0.298D-01-0.178D+00 0.955D-01

Coeff-Com: 0.277D+00 0.823D+00

Coeff: 0.469D-05-0.102D-03-0.904D-04-0.208D-03-0.143D-02 0.101D-02

Coeff: 0.429D-02 0.121D-01-0.265D-02-0.298D-01-0.178D+00 0.955D-01

Coeff: 0.277D+00 0.823D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=1.51D-08 MaxDP=7.39D-07 DE=-4.05D-11 OVMax= 1.14D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 6.29D-09 CP: 1.00D+00 1.01D+00 4.89D-01 7.85D-01 9.96D-01

CP: 1.18D+00 1.61D+00 1.83D+00 2.04D+00 2.63D+00

CP: 3.00D+00 2.59D+00 1.99D+00 1.60D+00

E= -1275.84253310289 Delta-E= -0.000000000046 Rises=F Damp=F

DIIS: error= 1.27D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.84253310289 IErMin=15 ErrMin= 1.27D-07

ErrMax= 1.27D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.14D-12 BMatP= 8.60D-12

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

Coeff-Com: -0.172D-05 0.177D-03 0.123D-03-0.314D-04-0.168D-02-0.507D-02

Coeff-Com: -0.135D-01 0.150D-01 0.455D-01 0.432D-01-0.271D-01-0.235D+00

Coeff-Com: -0.219D+00 0.357D+00 0.104D+01

Coeff: -0.172D-05 0.177D-03 0.123D-03-0.314D-04-0.168D-02-0.507D-02

Coeff: -0.135D-01 0.150D-01 0.455D-01 0.432D-01-0.271D-01-0.235D+00

Coeff: -0.219D+00 0.357D+00 0.104D+01

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=1.62D-08 MaxDP=8.06D-07 DE=-4.64D-11 OVMax= 1.24D-05

Cycle 16 Pass 1 IDiag 1:

RMSU= 2.58D-09 CP: 1.00D+00 1.01D+00 4.89D-01 7.85D-01 9.98D-01

CP: 1.18D+00 1.61D+00 1.85D+00 2.09D+00 2.77D+00

CP: 3.00D+00 3.00D+00 2.64D+00 2.66D+00 2.31D+00

E= -1275.84253310288 Delta-E= 0.000000000007 Rises=F Damp=F

DIIS: error= 7.72D-08 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=15 EnMin= -1275.84253310289 IErMin=16 ErrMin= 7.72D-08

ErrMax= 7.72D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.16D-12 BMatP= 4.14D-12

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

Coeff-Com: -0.300D-05 0.125D-03 0.863D-04 0.150D-03-0.118D-03-0.221D-02

Coeff-Com: -0.953D-02 0.106D-02 0.208D-01 0.397D-01 0.876D-01-0.170D+00

Coeff-Com: -0.272D+00-0.333D+00 0.674D+00 0.964D+00

Coeff: -0.300D-05 0.125D-03 0.863D-04 0.150D-03-0.118D-03-0.221D-02

Coeff: -0.953D-02 0.106D-02 0.208D-01 0.397D-01 0.876D-01-0.170D+00

Coeff: -0.272D+00-0.333D+00 0.674D+00 0.964D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=1.39D-08 MaxDP=7.21D-07 DE= 6.82D-12 OVMax= 1.07D-05

Cycle 17 Pass 1 IDiag 1:

RMSU= 7.19D-09 CP: 1.00D+00 1.01D+00 4.89D-01 7.84D-01 9.99D-01

CP: 1.18D+00 1.61D+00 1.86D+00 2.14D+00 2.88D+00

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

CP: 1.94D+00

E= -1275.84253310286 Delta-E= 0.000000000017 Rises=F Damp=F

DIIS: error= 3.23D-08 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=15 EnMin= -1275.84253310289 IErMin=17 ErrMin= 3.23D-08

ErrMax= 3.23D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.70D-13 BMatP= 2.16D-12

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

Coeff-Com: -0.681D-06-0.266D-04-0.238D-04 0.144D-03 0.789D-03 0.186D-02

Coeff-Com: 0.220D-02-0.684D-02-0.151D-01 0.796D-03 0.536D-01 0.378D-01

Coeff-Com: 0.482D-03-0.394D+00-0.175D+00 0.516D+00 0.978D+00

Coeff: -0.681D-06-0.266D-04-0.238D-04 0.144D-03 0.789D-03 0.186D-02

Coeff: 0.220D-02-0.684D-02-0.151D-01 0.796D-03 0.536D-01 0.378D-01

Coeff: 0.482D-03-0.394D+00-0.175D+00 0.516D+00 0.978D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=8.83D-09 MaxDP=4.54D-07 DE= 1.68D-11 OVMax= 6.73D-06

Error on total polarization charges = 0.06464

SCF Done: E(UB3LYP) = -1275.84253310 A.U. after 17 cycles

NFock= 17 Conv=0.88D-08 -V/T= 1.9659

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0176 S= 1.0059

<L.S>= 0.000000000000E+00

KE= 1.320816507000D+03 PE=-8.576820519835D+03 EE= 3.217751879721D+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 2.0176, after 2.0002

Leave Link 502 at Tue Sep 17 14:11:16 2019, MaxMem= 2415919104 cpu: 1520.2

(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= 15329 LenP2D= 41268.

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 = 247

Leave Link 701 at Tue Sep 17 14:11:20 2019, MaxMem= 2415919104 cpu: 70.5

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 14:11:20 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 14:11:30 2019, MaxMem= 2415919104 cpu: 178.6

(Enter /home/blab/g09/l716.exe)

Dipole = 1.70530257D-13-1.45217172D-13-2.22044605D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000203773 0.000448287 0.000000000

2 7 -0.001085364 -0.001992235 -0.000000000

3 6 0.000907397 0.002932594 -0.000000000

4 6 -0.003431654 -0.001386918 0.000000000

5 6 0.002795656 -0.001392262 -0.000000000

6 7 0.000457472 -0.001433085 0.000000000

7 6 -0.001021123 0.000788133 -0.000000000

8 7 0.001986565 -0.000095136 -0.000000000

9 6 -0.001908685 0.001129639 0.000000000

10 6 0.000702121 -0.003649328 -0.000000000

11 6 0.001885959 0.001768673 -0.000000000

12 7 -0.001634176 0.000332259 -0.000000000

13 6 -0.000702121 0.003649328 -0.000000000

14 6 -0.001885959 -0.001768673 0.000000000

15 6 0.001021123 -0.000788133 0.000000000

16 7 -0.001986565 0.000095136 -0.000000000

17 6 0.001908685 -0.001129639 0.000000000

18 7 -0.000457472 0.001433085 0.000000000

19 7 0.001085364 0.001992235 0.000000000

20 6 -0.000907397 -0.002932594 0.000000000

21 6 0.003431654 0.001386918 0.000000000

22 6 -0.002795656 0.001392262 -0.000000000

23 6 -0.000203773 -0.000448287 -0.000000000

24 7 0.001634176 -0.000332259 -0.000000000

25 30 -0.000000000 0.000000000 0.000000000

26 6 0.000146919 0.000359568 0.000000000

27 1 0.000167303 0.000261467 0.000000000

28 6 -0.000897731 -0.000184738 -0.000000000

29 1 -0.000033443 -0.000275810 0.000000000

30 6 0.000897731 0.000184738 -0.000000000

31 1 0.000033443 0.000275810 -0.000000000

32 6 -0.000146919 -0.000359568 0.000000000

33 1 -0.000167303 -0.000261467 -0.000000000

34 1 0.000224754 0.000025876 0.000000000

35 1 0.000064146 -0.000100445 -0.000559495

36 1 0.000064146 -0.000100445 0.000559495

37 1 0.000043879 0.000036853 -0.000560890

38 1 0.000043879 0.000036853 0.000560890

39 1 -0.000136811 0.000231040 0.000000000

40 1 -0.000043879 -0.000036853 -0.000560890

41 1 -0.000043879 -0.000036853 0.000560890

42 1 0.000136811 -0.000231040 0.000000000

43 1 -0.000064146 0.000100445 -0.000559495

44 1 -0.000064146 0.000100445 0.000559495

45 1 -0.000224754 -0.000025876 -0.000000000

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

Cartesian Forces: Max 0.003649328 RMS 0.001067520

Leave Link 716 at Tue Sep 17 14:11:30 2019, MaxMem= 2415919104 cpu: 0.4

(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 0.002051571 RMS 0.000475661

Search for a local minimum.

Step number 12 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 12

DE= -5.30D-04 DEPred=-7.26D-04 R= 7.31D-01

TightC=F SS= 1.41D+00 RLast= 8.79D-02 DXNew= 3.5676D-01 2.6380D-01

Trust test= 7.31D-01 RLast= 8.79D-02 DXMaxT set to 2.64D-01

ITU= 1 1 -1 0 1 -1 1 1 1 1 0 0

Eigenvalues --- 0.00809 0.00878 0.00878 0.00878 0.00878

Eigenvalues --- 0.01334 0.01335 0.01343 0.01344 0.01604

Eigenvalues --- 0.01623 0.01632 0.01640 0.01773 0.01792

Eigenvalues --- 0.01808 0.01821 0.01888 0.01908 0.01938

Eigenvalues --- 0.01949 0.01997 0.01999 0.02044 0.02047

Eigenvalues --- 0.02070 0.02086 0.02102 0.02110 0.02114

Eigenvalues --- 0.02205 0.02312 0.02316 0.02351 0.02373

Eigenvalues --- 0.03941 0.07229 0.07229 0.07229 0.07229

Eigenvalues --- 0.07316 0.07319 0.07395 0.08080 0.13613

Eigenvalues --- 0.14495 0.14504 0.15258 0.15669 0.15992

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16020 0.16218 0.16255 0.17147 0.18429

Eigenvalues --- 0.20538 0.22059 0.22091 0.23843 0.23856

Eigenvalues --- 0.23858 0.24353 0.24967 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25008

Eigenvalues --- 0.25255 0.28533 0.29022 0.31233 0.33108

Eigenvalues --- 0.33188 0.33198 0.33282 0.33282 0.33317

Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33745 0.33767 0.34340 0.34415

Eigenvalues --- 0.34437 0.34437 0.34445 0.35063 0.35557

Eigenvalues --- 0.35562 0.35633 0.35662 0.35682 0.35682

Eigenvalues --- 0.38549 0.41408 0.41631 0.41808 0.42772

Eigenvalues --- 0.46497 0.48032 0.48957 0.48981 0.51224

Eigenvalues --- 0.51359 0.51361 0.53257 0.53513 0.54010

Eigenvalues --- 0.54025 0.56320 0.56332 0.56519

Cosine: 0.387 < 0.560

Cut down GDIIS temporarily because of the cosine check. E 7

DIIS coeff's: 0.81659 1.57875 -0.69963 -1.52333 1.29134

DIIS coeff's: -0.46373

Cosine: 0.685 > 0.620

Length: 0.805

GDIIS step was calculated using 6 of the last 12 vectors.

Iteration 1 RMS(Cart)= 0.01340568 RMS(Int)= 0.00003947

Iteration 2 RMS(Cart)= 0.00009545 RMS(Int)= 0.00001234

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001234

ITry= 1 IFail=0 DXMaxC= 4.84D-02 DCOld= 1.00D+10 DXMaxT= 2.64D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.12D-09 for atom 43.

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

(Linear) (Quad) (Total)

R1 2.58261 0.00001 -0.00541 -0.01916 -0.02457 2.55804

R2 2.72863 0.00107 0.00026 0.01143 0.01166 2.74030

R3 2.58273 0.00159 0.01432 0.01085 0.02518 2.60791

R4 2.56477 -0.00053 0.00375 0.00663 0.01039 2.57516

R5 3.79364 0.00096 0.00394 0.00387 0.00782 3.80146

R6 2.76652 0.00147 -0.00580 0.00054 -0.00523 2.76128

R7 2.57843 0.00048 0.00694 -0.00433 0.00261 2.58104

R8 2.60338 -0.00189 0.00182 -0.00676 -0.00493 2.59845

R9 2.81417 -0.00003 0.00190 0.00272 0.00462 2.81879

R10 2.04359 -0.00028 -0.00125 -0.00044 -0.00169 2.04190

R11 2.49653 0.00045 -0.00397 -0.00582 -0.00979 2.48674

R12 2.58308 0.00004 0.00604 0.00978 0.01583 2.59891

R13 2.79708 0.00078 0.00448 -0.00249 0.00199 2.79907

R14 2.58058 -0.00050 -0.00395 -0.01847 -0.02243 2.55814

R15 3.77658 0.00108 0.00193 -0.00056 0.00137 3.77795

R16 2.83228 0.00176 0.01112 0.01557 0.02668 2.85896

R17 2.48670 0.00074 0.00113 0.00845 0.00957 2.49626

R18 2.55489 -0.00205 -0.00531 -0.00569 -0.01100 2.54388

R19 2.81011 -0.00087 -0.00322 -0.00224 -0.00546 2.80464

R20 2.04268 0.00022 0.00038 0.00468 0.00505 2.04773

R21 2.48670 0.00074 0.00113 0.00845 0.00957 2.49626

R22 2.55489 -0.00205 -0.00531 -0.00569 -0.01100 2.54388

R23 2.83228 0.00176 0.01112 0.01557 0.02668 2.85896

R24 2.81011 -0.00087 -0.00322 -0.00224 -0.00546 2.80464

R25 2.79708 0.00078 0.00448 -0.00249 0.00199 2.79907

R26 2.04268 0.00022 0.00038 0.00468 0.00505 2.04773

R27 2.58308 0.00004 0.00604 0.00978 0.01583 2.59891

R28 2.49653 0.00045 -0.00397 -0.00582 -0.00979 2.48674

R29 2.58058 -0.00050 -0.00395 -0.01847 -0.02243 2.55814

R30 3.77658 0.00108 0.00193 -0.00056 0.00137 3.77795

R31 2.57843 0.00048 0.00694 -0.00433 0.00261 2.58104

R32 2.56477 -0.00053 0.00375 0.00663 0.01039 2.57516

R33 2.58261 0.00001 -0.00541 -0.01916 -0.02457 2.55804

R34 3.79364 0.00096 0.00394 0.00387 0.00782 3.80146

R35 2.76652 0.00147 -0.00580 0.00054 -0.00523 2.76128

R36 2.60338 -0.00189 0.00182 -0.00676 -0.00493 2.59845

R37 2.81417 -0.00003 0.00190 0.00272 0.00462 2.81879

R38 2.72863 0.00107 0.00026 0.01143 0.01166 2.74030

R39 2.04359 -0.00028 -0.00125 -0.00044 -0.00169 2.04190

R40 2.58273 0.00159 0.01432 0.01085 0.02518 2.60791

R41 2.06290 -0.00019 -0.00074 0.00155 0.00081 2.06371

R42 2.07059 -0.00039 -0.00155 0.00316 0.00161 2.07220

R43 2.07059 -0.00039 -0.00155 0.00316 0.00161 2.07220

R44 2.06979 -0.00042 -0.00174 0.00405 0.00231 2.07210

R45 2.06979 -0.00042 -0.00174 0.00405 0.00231 2.07210

R46 2.06232 -0.00026 -0.00109 0.00097 -0.00011 2.06220

R47 2.06979 -0.00042 -0.00174 0.00405 0.00231 2.07210

R48 2.06979 -0.00042 -0.00174 0.00405 0.00231 2.07210

R49 2.06232 -0.00026 -0.00109 0.00097 -0.00011 2.06220

R50 2.07059 -0.00039 -0.00155 0.00316 0.00161 2.07220

R51 2.07059 -0.00039 -0.00155 0.00316 0.00161 2.07220

R52 2.06290 -0.00019 -0.00074 0.00155 0.00081 2.06371

A1 1.89546 -0.00075 0.00220 -0.00325 -0.00109 1.89436

A2 2.20517 0.00001 0.00008 -0.00230 -0.00220 2.20298

A3 2.18256 0.00074 -0.00228 0.00556 0.00329 2.18585

A4 1.90390 0.00042 -0.00142 -0.00189 -0.00333 1.90057

A5 2.18852 0.00028 0.00380 0.00701 0.01084 2.19936

A6 2.19077 -0.00070 -0.00238 -0.00512 -0.00751 2.18325

A7 1.89690 -0.00019 0.00069 0.00870 0.00942 1.90632

A8 2.21797 0.00093 -0.00161 -0.00139 -0.00300 2.21497

A9 2.16831 -0.00074 0.00092 -0.00732 -0.00642 2.16190

A10 1.85314 -0.00022 0.00059 -0.01318 -0.01256 1.84059

A11 2.17867 -0.00066 0.00176 0.00488 0.00662 2.18529

A12 2.25137 0.00089 -0.00235 0.00830 0.00594 2.25731

A13 1.87538 0.00074 -0.00205 0.00962 0.00756 1.88294

A14 2.18475 -0.00052 0.00210 -0.00542 -0.00332 2.18143

A15 2.22306 -0.00023 -0.00005 -0.00420 -0.00424 2.21882

A16 2.16884 -0.00040 0.00281 0.00748 0.01031 2.17915

A17 2.22961 0.00024 0.00086 -0.00066 0.00021 2.22982

A18 2.16992 -0.00036 0.00032 -0.00521 -0.00489 2.16502

A19 1.88366 0.00012 -0.00119 0.00587 0.00468 1.88835

A20 1.91198 0.00014 0.00046 0.00145 0.00193 1.91390

A21 2.19310 -0.00036 -0.00298 -0.00558 -0.00854 2.18455

A22 2.17811 0.00022 0.00252 0.00412 0.00662 2.18473

A23 1.88756 -0.00069 -0.00044 -0.00605 -0.00648 1.88109

A24 2.24374 0.00045 0.00458 0.00275 0.00731 2.25105

A25 2.15188 0.00023 -0.00414 0.00330 -0.00083 2.15105

A26 1.85497 0.00062 -0.00027 0.00879 0.00851 1.86347

A27 2.16038 -0.00087 -0.00137 -0.01105 -0.01241 2.14797

A28 2.26784 0.00025 0.00164 0.00225 0.00390 2.27175

A29 1.88661 -0.00021 0.00143 -0.01006 -0.00864 1.87797

A30 2.16696 -0.00007 -0.00164 0.00124 -0.00040 2.16657

A31 2.22961 0.00027 0.00021 0.00882 0.00904 2.23865

A32 2.17532 -0.00067 -0.00768 -0.00632 -0.01403 2.16130

A33 1.85497 0.00062 -0.00027 0.00879 0.00851 1.86347

A34 2.26784 0.00025 0.00164 0.00225 0.00390 2.27175

A35 2.16038 -0.00087 -0.00137 -0.01105 -0.01241 2.14797

A36 1.88661 -0.00021 0.00143 -0.01006 -0.00864 1.87797

A37 2.22961 0.00027 0.00021 0.00882 0.00904 2.23865

A38 2.16696 -0.00007 -0.00164 0.00124 -0.00040 2.16657

A39 1.88366 0.00012 -0.00119 0.00587 0.00468 1.88835

A40 2.16992 -0.00036 0.00032 -0.00521 -0.00489 2.16502

A41 2.22961 0.00024 0.00086 -0.00066 0.00021 2.22982

A42 1.91198 0.00014 0.00046 0.00145 0.00193 1.91390

A43 2.19310 -0.00036 -0.00298 -0.00558 -0.00854 2.18455

A44 2.17811 0.00022 0.00252 0.00412 0.00662 2.18473

A45 2.15188 0.00023 -0.00414 0.00330 -0.00083 2.15105

A46 2.24374 0.00045 0.00458 0.00275 0.00731 2.25105

A47 1.88756 -0.00069 -0.00044 -0.00605 -0.00648 1.88109

A48 2.16884 -0.00040 0.00281 0.00748 0.01031 2.17915

A49 1.90390 0.00042 -0.00142 -0.00189 -0.00333 1.90057

A50 2.19077 -0.00070 -0.00238 -0.00512 -0.00751 2.18325

A51 2.18852 0.00028 0.00380 0.00701 0.01084 2.19936

A52 2.21797 0.00093 -0.00161 -0.00139 -0.00300 2.21497

A53 2.16831 -0.00074 0.00092 -0.00732 -0.00642 2.16190

A54 1.89690 -0.00019 0.00069 0.00870 0.00942 1.90632

A55 1.85314 -0.00022 0.00059 -0.01318 -0.01256 1.84059

A56 2.17867 -0.00066 0.00176 0.00488 0.00662 2.18529

A57 2.25137 0.00089 -0.00235 0.00830 0.00594 2.25731

A58 1.87538 0.00074 -0.00205 0.00962 0.00756 1.88294

A59 2.22306 -0.00023 -0.00005 -0.00420 -0.00424 2.21882

A60 2.18475 -0.00052 0.00210 -0.00542 -0.00332 2.18143

A61 1.89546 -0.00075 0.00220 -0.00325 -0.00109 1.89436

A62 2.20517 0.00001 0.00008 -0.00230 -0.00220 2.20298

A63 2.18256 0.00074 -0.00228 0.00556 0.00329 2.18585

A64 2.17532 -0.00067 -0.00768 -0.00632 -0.01403 2.16130

A65 1.56609 0.00029 0.00330 0.00526 0.00854 1.57462

A66 1.57551 -0.00029 -0.00330 -0.00526 -0.00854 1.56697

A67 1.57551 -0.00029 -0.00330 -0.00526 -0.00854 1.56697

A68 1.56609 0.00029 0.00330 0.00526 0.00854 1.57462

A69 1.94022 0.00014 -0.00006 0.00122 0.00118 1.94140

A70 1.93958 0.00026 0.00165 0.00218 0.00382 1.94340

A71 1.93958 0.00026 0.00165 0.00218 0.00382 1.94340

A72 1.88939 -0.00010 -0.00028 -0.00008 -0.00034 1.88905

A73 1.88939 -0.00010 -0.00028 -0.00008 -0.00034 1.88905

A74 1.86288 -0.00050 -0.00286 -0.00578 -0.00870 1.85418

A75 1.93289 0.00021 -0.00036 0.00432 0.00397 1.93685

A76 1.93289 0.00021 -0.00036 0.00432 0.00397 1.93685

A77 1.94276 0.00005 0.00099 -0.00207 -0.00107 1.94169

A78 1.86315 -0.00043 -0.00337 -0.00641 -0.00978 1.85337

A79 1.89489 -0.00003 0.00148 -0.00024 0.00124 1.89613

A80 1.89489 -0.00003 0.00148 -0.00024 0.00124 1.89613

A81 1.93289 0.00021 -0.00036 0.00432 0.00397 1.93685

A82 1.93289 0.00021 -0.00036 0.00432 0.00397 1.93685

A83 1.94276 0.00005 0.00099 -0.00207 -0.00107 1.94169

A84 1.86315 -0.00043 -0.00337 -0.00641 -0.00978 1.85337

A85 1.89489 -0.00003 0.00148 -0.00024 0.00124 1.89613

A86 1.89489 -0.00003 0.00148 -0.00024 0.00124 1.89613

A87 1.93958 0.00026 0.00165 0.00218 0.00382 1.94340

A88 1.93958 0.00026 0.00165 0.00218 0.00382 1.94340

A89 1.94022 0.00014 -0.00006 0.00122 0.00118 1.94140

A90 1.86288 -0.00050 -0.00286 -0.00578 -0.00870 1.85418

A91 1.88939 -0.00010 -0.00028 -0.00008 -0.00034 1.88905

A92 1.88939 -0.00010 -0.00028 -0.00008 -0.00034 1.88905

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 1.03591 -0.00014 -0.00080 -0.00220 -0.00297 1.03293

D31 -1.03591 0.00014 0.00080 0.00220 0.00297 -1.03293

D32 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.10569 -0.00014 -0.00080 -0.00220 -0.00297 -2.10866

D34 2.10569 0.00014 0.00080 0.00220 0.00297 2.10866

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

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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

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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

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D57 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

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D63 1.03177 -0.00013 -0.00232 -0.00124 -0.00356 1.02820

D64 -1.03177 0.00013 0.00232 0.00124 0.00356 -1.02820

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D79 -2.10983 -0.00013 -0.00232 -0.00124 -0.00356 -2.11339

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D90 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

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D111 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

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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

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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

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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 1.03591 -0.00014 -0.00080 -0.00220 -0.00297 1.03293

D126 -1.03591 0.00014 0.00080 0.00220 0.00297 -1.03293

D127 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

D128 -2.10569 -0.00014 -0.00080 -0.00220 -0.00297 -2.10866

D129 2.10569 0.00014 0.00080 0.00220 0.00297 2.10866

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 0.002052 0.000450 NO

RMS Force 0.000476 0.000300 NO

Maximum Displacement 0.048413 0.001800 NO

RMS Displacement 0.013406 0.001200 NO

Predicted change in Energy=-1.908944D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:11:30 2019, MaxMem= 2415919104 cpu: 1.3

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.063568 -2.196142 0.000000

2 7 0 -0.750705 -1.866324 0.000000

3 6 0 -0.008579 -3.009233 0.000000

4 6 0 -0.903743 -4.164141 0.000000

5 6 0 -2.175750 -3.641900 0.000000

6 7 0 1.354065 -3.102406 0.000000

7 6 0 2.178053 -2.076389 0.000000

8 7 0 1.857623 -0.738955 0.000000

9 6 0 2.991239 0.000941 0.000000

10 6 0 4.165488 -0.952996 0.000000

11 6 0 3.654230 -2.198297 0.000000

12 7 0 -3.125733 -1.315042 0.000000

13 6 0 -4.165488 0.952996 0.000000

14 6 0 -3.654230 2.198297 0.000000

15 6 0 -2.178053 2.076389 0.000000

16 7 0 -1.857623 0.738955 0.000000

17 6 0 -2.991239 -0.000941 0.000000

18 7 0 -1.354065 3.102406 0.000000

19 7 0 0.750705 1.866324 0.000000

20 6 0 0.008579 3.009233 0.000000

21 6 0 0.903743 4.164141 0.000000

22 6 0 2.175750 3.641900 0.000000

23 6 0 2.063568 2.196142 0.000000

24 7 0 3.125733 1.315042 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.467309 -5.590506 0.000000

27 1 0 -3.106290 -4.191115 0.000000

28 6 0 5.578270 -0.498291 0.000000

29 1 0 4.186414 -3.142224 0.000000

30 6 0 -5.578270 0.498291 0.000000

31 1 0 -4.186414 3.142224 0.000000

32 6 0 0.467309 5.590506 0.000000

33 1 0 3.106290 4.191115 0.000000

34 1 0 -1.324967 -6.266553 0.000000

35 1 0 0.149814 -5.819141 0.877113

36 1 0 0.149814 -5.819141 -0.877113

37 1 0 5.789905 0.125209 0.876806

38 1 0 5.789905 0.125209 -0.876806

39 1 0 6.266382 -1.345271 0.000000

40 1 0 -5.789905 -0.125209 0.876806

41 1 0 -5.789905 -0.125209 -0.876806

42 1 0 -6.266382 1.345271 0.000000

43 1 0 -0.149814 5.819141 0.877113

44 1 0 -0.149814 5.819141 -0.877113

45 1 0 1.324967 6.266553 0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.353658 0.000000

3 C 2.209999 1.362715 0.000000

4 C 2.284341 2.302907 1.461208 0.000000

5 C 1.450104 2.276713 2.257631 1.375042 0.000000

6 N 3.535750 2.440892 1.365826 2.494990 3.570805

7 C 4.243311 2.936282 2.377300 3.722388 4.626708

8 N 4.183196 2.841538 2.938856 4.399663 4.969425

9 C 5.511646 4.181964 4.249712 5.702525 6.322030

10 C 6.351893 5.000312 4.653058 6.000713 6.887780

11 C 5.717798 4.417426 3.751504 4.963835 6.006052

12 N 1.380047 2.438169 3.547806 3.613115 2.513311

13 C 3.786177 4.428240 5.742748 6.068284 5.007207

14 C 4.673467 4.995158 6.356818 6.931507 6.024433

15 C 4.274065 4.193127 5.529030 6.369308 5.718289

16 N 2.942313 2.830679 4.179459 4.995021 4.392390

17 C 2.383166 2.915415 4.236281 4.657238 3.731166

18 N 5.345840 5.005230 6.257992 7.280487 6.794176

19 N 4.942040 4.023294 4.934325 6.253295 6.237361

20 C 5.602653 4.934325 6.018490 7.231156 7.000633

21 C 7.018413 6.253295 7.231156 8.522163 8.391516

22 C 7.214883 6.237361 7.000633 8.391516 8.484650

23 C 6.027056 4.942040 5.602653 7.018413 7.214883

24 N 6.265561 5.014764 5.340718 6.801332 7.257892

25 Zn 3.013528 2.011647 3.009245 4.261082 4.242325

26 C 3.750967 3.734949 2.621718 1.491641 2.591494

27 H 2.251041 3.309597 3.315518 2.202712 1.080528

28 C 7.828179 6.475140 6.125170 7.446808 8.367025

29 H 6.321182 5.099320 4.197101 5.191725 6.381756

30 C 4.428668 5.375573 6.582111 6.602232 5.358947

31 H 5.744966 6.073686 7.436043 8.009925 7.075811

32 C 8.187626 7.555652 8.612896 9.850529 9.603285

33 H 8.217328 7.181154 7.845216 9.267721 9.447543

34 H 4.136881 4.437544 3.513262 2.144194 2.759101

35 H 4.335264 4.147894 2.947881 2.149032 3.304233

36 H 4.335264 4.147894 2.947881 2.149032 3.304233

37 H 8.236170 6.893081 6.649506 7.998264 8.855030

38 H 8.236170 6.893081 6.649506 7.998264 8.855030

39 H 8.373293 7.036405 6.491833 7.704330 8.748948

40 H 4.352372 5.403129 6.519978 6.399714 5.118399

41 H 4.352372 5.403129 6.519978 6.399714 5.118399

42 H 5.495930 6.382557 7.623765 7.688401 6.450204

43 H 8.287131 7.758658 8.872962 10.050057 9.715196

44 H 8.287131 7.758658 8.872962 10.050057 9.715196

45 H 9.115886 8.393575 9.371155 10.666139 10.508685

6 7 8 9 10

6 N 0.000000

7 C 1.315928 0.000000

8 N 2.416500 1.375284 0.000000

9 C 3.508718 2.230823 1.353710 0.000000

10 C 3.538936 2.282961 2.317769 1.512897 0.000000

11 C 2.471472 1.481202 2.314622 2.296999 1.346165

12 N 4.823200 5.358152 5.016544 6.256928 7.300204

13 C 6.849216 7.029772 6.256242 7.219775 8.546226

14 C 7.292494 7.231076 6.245636 6.999331 8.430815

15 C 6.268635 6.018407 4.920655 5.570374 7.029772

16 N 5.007094 4.920655 3.998408 4.904705 6.256242

17 C 5.338610 5.570374 4.904705 5.982478 7.219775

18 N 6.770057 6.268635 5.007094 5.338610 6.849216

19 N 5.005230 4.193127 2.830679 2.915415 4.428240

20 C 6.257992 5.529030 4.179459 4.236281 5.742748

21 C 7.280487 6.369308 4.995021 4.657238 6.068284

22 C 6.794176 5.718289 4.392390 3.731166 5.007207

23 C 5.345840 4.274065 2.942313 2.383166 3.786177

24 N 4.759481 3.521350 2.413919 1.320966 2.495013

25 Zn 3.385028 3.009204 1.999204 2.991239 4.273113

26 C 3.083512 4.398518 5.379857 6.574636 6.555098

27 H 4.591302 5.691779 6.046308 7.399540 7.960162

28 C 4.962391 3.748583 3.728422 2.634760 1.484153

29 H 2.832629 2.273658 3.346487 3.362727 2.189329

30 C 7.811676 8.172486 7.538122 8.583929 9.851246

31 H 8.348193 8.230454 7.182892 7.834945 9.301887

32 C 8.738024 7.855440 6.480359 6.132982 7.516246

33 H 7.501049 6.335869 5.085740 4.191753 5.252026

34 H 4.145966 5.461558 6.378340 7.609935 7.640614

35 H 3.098418 4.346409 5.430859 6.535777 6.369799

36 H 3.098418 4.346409 5.430859 6.535777 6.369799

37 H 5.555445 4.319872 4.120486 2.935432 2.137766

38 H 5.555445 4.319872 4.120486 2.935432 2.137766

39 H 5.217124 4.153187 4.450255 3.541023 2.137202

40 H 7.789018 8.250106 7.722056 8.825712 10.028154

41 H 7.789018 8.250106 7.722056 8.825712 10.028154

42 H 8.823437 9.111324 8.387100 9.354719 10.682038

43 H 9.089829 8.278146 6.914315 6.669857 8.077933

44 H 9.089829 8.278146 6.914315 6.669857 8.077933

45 H 9.369005 8.386444 7.025729 6.483391 7.758250

11 12 13 14 15

11 C 0.000000

12 N 6.837253 0.000000

13 C 8.430815 2.495013 0.000000

14 C 8.528987 3.552867 1.346165 0.000000

15 C 7.231076 3.521350 2.282961 1.481202 0.000000

16 N 6.245636 2.413919 2.317769 2.314622 1.375284

17 C 6.999331 1.320966 1.512897 2.296999 2.230823

18 N 7.292494 4.759481 3.538936 2.471472 1.315928

19 N 4.995158 5.014764 5.000312 4.417426 2.936282

20 C 6.356818 5.340718 4.653058 3.751504 2.377300

21 C 6.931507 6.801332 6.000713 4.963835 3.722388

22 C 6.024433 7.257892 6.887780 6.006052 4.626708

23 C 4.673467 6.265561 6.351893 5.717798 4.243311

24 N 3.552867 6.782195 7.300204 6.837253 5.358152

25 Zn 4.264494 3.391097 4.273113 4.264494 3.009204

26 C 5.337993 5.034562 7.516246 8.415576 7.855440

27 H 7.048117 2.876138 5.252026 6.412864 6.335869

28 C 2.567479 8.742239 9.851246 9.618245 8.172486

29 H 1.083614 7.536981 9.301887 9.486668 8.230454

30 C 9.618245 3.050101 1.484153 2.567479 3.748583

31 H 9.486668 4.581732 2.189329 1.083614 2.273658

32 C 8.415576 7.784378 6.555098 5.337993 4.398518

33 H 6.412864 8.316001 7.960162 7.048117 5.691779

34 H 6.429861 5.268797 7.758250 8.779474 8.386444

35 H 5.114760 5.637858 8.077933 8.917365 8.278146

36 H 5.114760 5.637858 8.077933 8.917365 8.278146

37 H 3.275451 9.073682 10.028154 9.708664 8.250106

38 H 3.275451 9.073682 10.028154 9.708664 8.250106

39 H 2.747906 9.392163 10.682038 10.534487 9.111324

40 H 9.708664 3.046687 2.137766 3.275451 4.319872

41 H 9.708664 3.046687 2.137766 3.275451 4.319872

42 H 10.534487 4.115938 2.137202 2.747906 4.153187

43 H 8.917365 7.779588 6.369799 5.114760 4.346409

44 H 8.917365 7.779588 6.369799 5.114760 4.346409

45 H 8.779474 8.791434 7.640614 6.429861 5.461558

16 17 18 19 20

16 N 0.000000

17 C 1.353710 0.000000

18 N 2.416500 3.508718 0.000000

19 N 2.841538 4.181964 2.440892 0.000000

20 C 2.938856 4.249712 1.365826 1.362715 0.000000

21 C 4.399663 5.702525 2.494990 2.302907 1.461208

22 C 4.969425 6.322030 3.570805 2.276713 2.257631

23 C 4.183196 5.511646 3.535750 1.353658 2.209999

24 N 5.016544 6.256928 4.823200 2.438169 3.547806

25 Zn 1.999204 2.991239 3.385028 2.011647 3.009245

26 C 6.480359 6.132982 8.738024 7.555652 8.612896

27 H 5.085740 4.191753 7.501049 7.181154 7.845216

28 C 7.538122 8.583929 7.811676 5.375573 6.582111

29 H 7.182892 7.834945 8.348193 6.073686 7.436043

30 C 3.728422 2.634760 4.962391 6.475140 6.125170

31 H 3.346487 3.362727 2.832629 5.099320 4.197101

32 C 5.379857 6.574636 3.083512 3.734949 2.621718

33 H 6.046308 7.399540 4.591302 3.309597 3.315518

34 H 7.025729 6.483391 9.369005 8.393575 9.371155

35 H 6.914315 6.669857 9.089829 7.758658 8.872962

36 H 6.914315 6.669857 9.089829 7.758658 8.872962

37 H 7.722056 8.825712 7.789018 5.403129 6.519978

38 H 7.722056 8.825712 7.789018 5.403129 6.519978

39 H 8.387100 9.354719 8.823437 6.382557 7.623765

40 H 4.120486 2.935432 5.555445 6.893081 6.649506

41 H 4.120486 2.935432 5.555445 6.893081 6.649506

42 H 4.450255 3.541023 5.217124 7.036405 6.491833

43 H 5.430859 6.535777 3.098418 4.147894 2.947881

44 H 5.430859 6.535777 3.098418 4.147894 2.947881

45 H 6.378340 7.609935 4.145966 4.437544 3.513262

21 22 23 24 25

21 C 0.000000

22 C 1.375042 0.000000

23 C 2.284341 1.450104 0.000000

24 N 3.613115 2.513311 1.380047 0.000000

25 Zn 4.261082 4.242325 3.013528 3.391097 0.000000

26 C 9.850529 9.603285 8.187626 7.784378 5.610003

27 H 9.267721 9.447543 8.217328 8.316001 5.216750

28 C 6.602232 5.358947 4.428668 3.050101 5.600481

29 H 8.009925 7.075811 5.744966 4.581732 5.234466

30 C 7.446808 8.367025 7.828179 8.742239 5.600481

31 H 5.191725 6.381756 6.321182 7.536981 5.234466

32 C 1.491641 2.591494 3.750967 5.034562 5.610003

33 H 2.202712 1.080528 2.251041 2.876138 5.216750

34 H 10.666139 10.508685 9.115886 8.791434 6.405094

35 H 10.050057 9.715196 8.287131 7.779588 5.886780

36 H 10.050057 9.715196 8.287131 7.779588 5.886780

37 H 6.399714 5.118399 4.352372 3.046687 5.857257

38 H 6.399714 5.118399 4.352372 3.046687 5.857257

39 H 7.688401 6.450204 5.495930 4.115938 6.409157

40 H 7.998264 8.855030 8.236170 9.073682 5.857257

41 H 7.998264 8.855030 8.236170 9.073682 5.857257

42 H 7.704330 8.748948 8.373293 9.392163 6.409157

43 H 2.149032 3.304233 4.335264 5.637858 5.886780

44 H 2.149032 3.304233 4.335264 5.637858 5.886780

45 H 2.144194 2.759101 4.136881 5.268797 6.405094

26 27 28 29 30

26 C 0.000000

27 H 2.987059 0.000000

28 C 7.904409 9.437083 0.000000

29 H 5.258443 7.367748 2.987917 0.000000

30 C 7.949552 5.301058 11.200963 10.421248 0.000000

31 H 9.491698 7.412458 10.421248 10.468933 2.987917

32 C 11.220007 10.413967 7.949552 9.491698 7.904409

33 H 10.413967 10.433500 5.301058 7.412458 9.437083

34 H 1.092070 2.735061 8.995973 6.335357 7.990851

35 H 1.096559 3.744597 7.651726 4.922332 8.572644

36 H 1.096559 3.744597 7.651726 4.922332 8.572644

37 H 8.520030 9.926818 1.096508 3.743807 11.408040

38 H 8.520030 9.926818 1.096508 3.743807 11.408040

39 H 7.960189 9.795193 1.091271 2.748692 11.987264

40 H 7.679081 4.949966 11.408040 10.459355 1.096508

41 H 7.679081 4.949966 11.408040 10.459355 1.096508

42 H 9.040700 6.374774 11.987264 11.375349 1.091271

43 H 11.447715 10.474507 8.572644 9.993912 7.651726

44 H 11.447715 10.474507 8.572644 9.993912 7.651726

45 H 11.991752 11.357766 7.990851 9.834276 8.995973

31 32 33 34 35

31 H 0.000000

32 C 5.258443 0.000000

33 H 7.367748 2.987059 0.000000

34 H 9.834276 11.991752 11.357766 0.000000

35 H 9.993912 11.447715 10.474507 1.773269 0.000000

36 H 9.993912 11.447715 10.474507 1.773269 1.754227

37 H 10.459355 7.679081 4.949966 9.604416 8.194262

38 H 10.459355 7.679081 4.949966 9.604416 8.379866

39 H 11.375349 9.040700 6.374774 9.046966 7.628712

40 H 3.743807 8.520030 9.926818 7.643335 8.228069

41 H 3.743807 8.520030 9.926818 7.643335 8.412928

42 H 2.748692 7.960189 9.795193 9.075101 9.657417

43 H 4.922332 1.096559 3.744597 12.174330 11.642139

44 H 4.922332 1.096559 3.744597 12.174330 11.773559

45 H 6.335357 1.092070 2.735061 12.810188 12.174330

36 37 38 39 40

36 H 0.000000

37 H 8.379866 0.000000

38 H 8.194262 1.753612 0.000000

39 H 7.628712 1.777113 1.777113 0.000000

40 H 8.412928 11.582517 11.714515 12.149542 0.000000

41 H 8.228069 11.714515 11.582517 12.149542 1.753612

42 H 9.657417 12.149542 12.149542 12.818314 1.777113

43 H 11.773559 8.228069 8.412928 9.657417 8.194262

44 H 11.642139 8.412928 8.228069 9.657417 8.379866

45 H 12.174330 7.643335 7.643335 9.075101 9.604416

41 42 43 44 45

41 H 0.000000

42 H 1.777113 0.000000

43 H 8.379866 7.628712 0.000000

44 H 8.194262 7.628712 1.754227 0.000000

45 H 9.604416 9.046966 1.773269 1.773269 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=0 Diff= 1.07D+00

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 2.769768 1.187322 0.000000

2 7 0 1.434586 1.410208 0.000000

3 6 0 1.211603 2.754555 0.000000

4 6 0 2.494010 3.454958 0.000000

5 6 0 3.450911 2.467496 0.000000

6 7 0 0.000000 3.385028 0.000000

7 6 0 -1.165615 2.774284 0.000000

8 7 0 -1.406933 1.420337 0.000000

9 6 0 -2.741872 1.195680 0.000000

10 6 0 -3.436491 2.539690 0.000000

11 6 0 -2.469778 3.476507 0.000000

12 7 0 3.390797 -0.045096 0.000000

13 6 0 3.436491 -2.539690 0.000000

14 6 0 2.469778 -3.476507 0.000000

15 6 0 1.165615 -2.774284 0.000000

16 7 0 1.406933 -1.420337 0.000000

17 6 0 2.741872 -1.195680 0.000000

18 7 0 -0.000000 -3.385028 0.000000

19 7 0 -1.434586 -1.410208 0.000000

20 6 0 -1.211603 -2.754555 0.000000

21 6 0 -2.494010 -3.454958 0.000000

22 6 0 -3.450911 -2.467496 0.000000

23 6 0 -2.769768 -1.187322 0.000000

24 7 0 -3.390797 0.045096 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 2.664583 4.936814 0.000000

27 1 0 4.523453 2.598626 0.000000

28 6 0 -4.913206 2.688084 0.000000

29 1 0 -2.579944 4.554507 0.000000

30 6 0 4.913206 -2.688084 0.000000

31 1 0 2.579944 -4.554507 0.000000

32 6 0 -2.664583 -4.936814 0.000000

33 1 0 -4.523453 -2.598626 0.000000

34 1 0 3.721063 5.213340 0.000000

35 1 0 2.190443 5.393219 0.877113

36 1 0 2.190443 5.393219 -0.877113

37 1 0 -5.356581 2.201298 0.876806

38 1 0 -5.356581 2.201298 -0.876806

39 1 0 -5.205061 3.739604 0.000000

40 1 0 5.356581 -2.201298 0.876806

41 1 0 5.356581 -2.201298 -0.876806

42 1 0 5.205061 -3.739604 0.000000

43 1 0 -2.190443 -5.393219 0.877113

44 1 0 -2.190443 -5.393219 -0.877113

45 1 0 -3.721063 -5.213340 0.000000

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

Rotational constants (GHZ): 0.1831806 0.1813381 0.0913316

Leave Link 202 at Tue Sep 17 14:11:30 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 101 beta electrons

nuclear repulsion energy 2760.6652941099 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= -0.1140425006 Hartrees.

Nuclear repulsion after empirical dispersion term = 2760.5512516093 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 = 3572

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.15D-07

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 226

GePol: Fraction of low-weight points (<1% of avg) = 6.33%

GePol: Cavity surface area = 378.537 Ang\*\*2

GePol: Cavity volume = 378.307 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0106882098 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2760.5405633995 Hartrees.

Leave Link 301 at Tue Sep 17 14:11:30 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= 15315 LenP2D= 41258.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.85D-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 14:11:31 2019, MaxMem= 2415919104 cpu: 12.5

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:11:31 2019, MaxMem= 2415919104 cpu: 1.6

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.925515 -0.000000 -0.000000 -0.378710 Ang= -44.51 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 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0176 S= 1.0058

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= -1276.14705479742

Leave Link 401 at Tue Sep 17 14:11:33 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= 38277552.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.88D-15 for 3570.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.88D-15 for 3570 1329.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.11D-15 for 3570.

Iteration 1 A^-1\*A deviation from orthogonality is 8.68D-12 for 2008 1979.

E= -1275.84095075985

DIIS: error= 1.01D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.84095075985 IErMin= 1 ErrMin= 1.01D-03

ErrMax= 1.01D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.80D-03 BMatP= 3.80D-03

IDIUse=3 WtCom= 9.90D-01 WtEn= 1.01D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.304 Goal= None Shift= 0.000

Gap= 0.393 Goal= None Shift= 0.000

GapD= 0.304 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.

RMSDP=1.15D-04 MaxDP=3.77D-03 OVMax= 2.90D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.15D-04 CP: 1.00D+00

E= -1275.84236307051 Delta-E= -0.001412310663 Rises=F Damp=F

DIIS: error= 6.53D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84236307051 IErMin= 2 ErrMin= 6.53D-04

ErrMax= 6.53D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.62D-04 BMatP= 3.80D-03

IDIUse=3 WtCom= 9.93D-01 WtEn= 6.53D-03

Coeff-Com: 0.101D+00 0.899D+00

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

Coeff: 0.101D+00 0.899D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.11D-05 MaxDP=2.20D-03 DE=-1.41D-03 OVMax= 2.59D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.98D-05 CP: 1.00D+00 1.09D+00

E= -1275.84236995061 Delta-E= -0.000006880098 Rises=F Damp=F

DIIS: error= 9.70D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1275.84236995061 IErMin= 2 ErrMin= 6.53D-04

ErrMax= 9.70D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.55D-04 BMatP= 3.62D-04

IDIUse=3 WtCom= 2.43D-01 WtEn= 7.57D-01

Coeff-Com: -0.137D-01 0.606D+00 0.408D+00

Coeff-En: 0.000D+00 0.485D+00 0.515D+00

Coeff: -0.333D-02 0.515D+00 0.489D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.76D-05 MaxDP=1.47D-03 DE=-6.88D-06 OVMax= 5.87D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.34D-05 CP: 1.00D+00 1.17D+00 7.08D-01

E= -1275.84253339735 Delta-E= -0.000163446738 Rises=F Damp=F

DIIS: error= 5.28D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84253339735 IErMin= 4 ErrMin= 5.28D-04

ErrMax= 5.28D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.05D-04 BMatP= 3.62D-04

IDIUse=3 WtCom= 9.95D-01 WtEn= 5.28D-03

Coeff-Com: -0.749D-02 0.108D+00 0.279D+00 0.620D+00

Coeff-En: 0.000D+00 0.000D+00 0.688D-01 0.931D+00

Coeff: -0.745D-02 0.107D+00 0.278D+00 0.622D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.75D-05 MaxDP=9.81D-04 DE=-1.63D-04 OVMax= 1.19D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 7.20D-06 CP: 1.00D+00 1.19D+00 1.10D+00 1.06D+00

E= -1275.84258552799 Delta-E= -0.000052130649 Rises=F Damp=F

DIIS: error= 2.47D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84258552799 IErMin= 5 ErrMin= 2.47D-04

ErrMax= 2.47D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.80D-05 BMatP= 1.05D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.47D-03

Coeff-Com: 0.176D-03-0.613D-01 0.419D-01 0.357D+00 0.662D+00

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

Coeff: 0.175D-03-0.611D-01 0.418D-01 0.357D+00 0.663D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.32D-05 MaxDP=5.97D-04 DE=-5.21D-05 OVMax= 9.59D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.41D-06 CP: 1.00D+00 1.24D+00 1.31D+00 1.41D+00 1.28D+00

E= -1275.84261126137 Delta-E= -0.000025733372 Rises=F Damp=F

DIIS: error= 2.00D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84261126137 IErMin= 6 ErrMin= 2.00D-04

ErrMax= 2.00D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.27D-06 BMatP= 1.80D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.00D-03

Coeff-Com: 0.106D-01-0.143D+00-0.294D+00-0.345D+00 0.256D+00 0.152D+01

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

Coeff: 0.106D-01-0.143D+00-0.293D+00-0.344D+00 0.255D+00 0.151D+01

Gap= 0.055 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.10D-05 MaxDP=1.57D-03 DE=-2.57D-05 OVMax= 2.33D-02

Cycle 7 Pass 1 IDiag 1:

RMSU= 3.99D-06 CP: 1.00D+00 1.33D+00 1.83D+00 2.15D+00 2.48D+00

CP: 2.24D+00

E= -1275.84264791630 Delta-E= -0.000036654936 Rises=F Damp=F

DIIS: error= 1.08D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84264791630 IErMin= 7 ErrMin= 1.08D-04

ErrMax= 1.08D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.82D-06 BMatP= 8.27D-06

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.08D-03

Coeff-Com: 0.791D-02-0.742D-01-0.249D+00-0.413D+00-0.110D+00 0.113D+01

Coeff-Com: 0.710D+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: 0.790D-02-0.741D-01-0.248D+00-0.412D+00-0.110D+00 0.113D+01

Coeff: 0.711D+00

Gap= 0.055 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.73D-05 MaxDP=8.48D-04 DE=-3.67D-05 OVMax= 1.28D-02

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.48D-06 CP: 1.00D+00 1.38D+00 2.12D+00 2.57D+00 3.00D+00

CP: 3.00D+00 1.30D+00

E= -1275.84265658330 Delta-E= -0.000008666993 Rises=F Damp=F

DIIS: error= 3.00D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84265658330 IErMin= 8 ErrMin= 3.00D-05

ErrMax= 3.00D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.34D-07 BMatP= 4.82D-06

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

Coeff-Com: -0.139D-02 0.426D-01 0.259D-01-0.968D-02-0.104D+00-0.173D+00

Coeff-Com: 0.285D+00 0.934D+00

Coeff: -0.139D-02 0.426D-01 0.259D-01-0.968D-02-0.104D+00-0.173D+00

Coeff: 0.285D+00 0.934D+00

Gap= 0.055 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.50D-06 MaxDP=2.57D-04 DE=-8.67D-06 OVMax= 3.33D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.85D-06 CP: 1.00D+00 1.39D+00 2.19D+00 2.66D+00 3.00D+00

CP: 3.00D+00 1.62D+00 1.63D+00

E= -1275.84265760670 Delta-E= -0.000001023408 Rises=F Damp=F

DIIS: error= 1.38D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84265760670 IErMin= 9 ErrMin= 1.38D-05

ErrMax= 1.38D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.39D-07 BMatP= 7.34D-07

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

Coeff-Com: -0.194D-02 0.332D-01 0.560D-01 0.691D-01-0.784D-02-0.289D+00

Coeff-Com: -0.284D-01 0.437D+00 0.732D+00

Coeff: -0.194D-02 0.332D-01 0.560D-01 0.691D-01-0.784D-02-0.289D+00

Coeff: -0.284D-01 0.437D+00 0.732D+00

Gap= 0.055 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.19D-06 MaxDP=5.87D-05 DE=-1.02D-06 OVMax= 7.30D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 4.91D-07 CP: 1.00D+00 1.39D+00 2.20D+00 2.68D+00 3.00D+00

CP: 3.00D+00 1.72D+00 1.90D+00 1.21D+00

E= -1275.84265779740 Delta-E= -0.000000190696 Rises=F Damp=F

DIIS: error= 7.69D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84265779740 IErMin=10 ErrMin= 7.69D-06

ErrMax= 7.69D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.28D-08 BMatP= 2.39D-07

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

Coeff-Com: -0.483D-03 0.225D-02 0.164D-01 0.341D-01 0.299D-01-0.841D-01

Coeff-Com: -0.108D+00-0.268D-01 0.366D+00 0.771D+00

Coeff: -0.483D-03 0.225D-02 0.164D-01 0.341D-01 0.299D-01-0.841D-01

Coeff: -0.108D+00-0.268D-01 0.366D+00 0.771D+00

Gap= 0.055 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=8.76D-07 MaxDP=5.14D-05 DE=-1.91D-07 OVMax= 6.15D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 3.09D-07 CP: 1.00D+00 1.39D+00 2.21D+00 2.69D+00 3.00D+00

CP: 3.00D+00 1.78D+00 2.04D+00 1.38D+00 1.19D+00

E= -1275.84265786865 Delta-E= -0.000000071247 Rises=F Damp=F

DIIS: error= 6.12D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84265786865 IErMin=11 ErrMin= 6.12D-06

ErrMax= 6.12D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.21D-08 BMatP= 6.28D-08

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

Coeff-Com: 0.179D-03-0.594D-02-0.416D-02 0.500D-02 0.137D-01 0.220D-01

Coeff-Com: -0.549D-01-0.939D-01-0.173D-01 0.352D+00 0.784D+00

Coeff: 0.179D-03-0.594D-02-0.416D-02 0.500D-02 0.137D-01 0.220D-01

Coeff: -0.549D-01-0.939D-01-0.173D-01 0.352D+00 0.784D+00

Gap= 0.055 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.90D-07 MaxDP=2.37D-05 DE=-7.12D-08 OVMax= 3.26D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.59D-07 CP: 1.00D+00 1.39D+00 2.22D+00 2.70D+00 3.00D+00

CP: 3.00D+00 1.81D+00 2.11D+00 1.45D+00 1.52D+00

CP: 1.31D+00

E= -1275.84265789247 Delta-E= -0.000000023822 Rises=F Damp=F

DIIS: error= 2.52D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84265789247 IErMin=12 ErrMin= 2.52D-06

ErrMax= 2.52D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.09D-08 BMatP= 2.21D-08

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

Coeff-Com: 0.312D-03-0.497D-02-0.102D-01-0.102D-01-0.537D-02 0.502D-01

Coeff-Com: 0.225D-02-0.443D-01-0.173D+00-0.704D-01 0.541D+00 0.725D+00

Coeff: 0.312D-03-0.497D-02-0.102D-01-0.102D-01-0.537D-02 0.502D-01

Coeff: 0.225D-02-0.443D-01-0.173D+00-0.704D-01 0.541D+00 0.725D+00

Gap= 0.055 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.86D-07 MaxDP=2.67D-05 DE=-2.38D-08 OVMax= 3.58D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 9.62D-08 CP: 1.00D+00 1.39D+00 2.22D+00 2.71D+00 3.00D+00

CP: 3.00D+00 1.83D+00 2.17D+00 1.53D+00 1.69D+00

CP: 1.67D+00 1.09D+00

E= -1275.84265790431 Delta-E= -0.000000011844 Rises=F Damp=F

DIIS: error= 1.36D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84265790431 IErMin=13 ErrMin= 1.36D-06

ErrMax= 1.36D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.39D-09 BMatP= 1.09D-08

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

Coeff-Com: 0.615D-04 0.489D-04-0.249D-02-0.472D-02-0.608D-02 0.109D-01

Coeff-Com: 0.128D-01 0.154D-01-0.602D-01-0.120D+00-0.300D-01 0.253D+00

Coeff-Com: 0.932D+00

Coeff: 0.615D-04 0.489D-04-0.249D-02-0.472D-02-0.608D-02 0.109D-01

Coeff: 0.128D-01 0.154D-01-0.602D-01-0.120D+00-0.300D-01 0.253D+00

Coeff: 0.932D+00

Gap= 0.055 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.59D-07 MaxDP=1.29D-05 DE=-1.18D-08 OVMax= 1.89D-04

Cycle 14 Pass 1 IDiag 1:

RMSU= 3.98D-08 CP: 1.00D+00 1.40D+00 2.23D+00 2.71D+00 3.00D+00

CP: 3.00D+00 1.84D+00 2.21D+00 1.56D+00 1.79D+00

CP: 1.83D+00 1.36D+00 1.30D+00

E= -1275.84265790625 Delta-E= -0.000000001941 Rises=F Damp=F

DIIS: error= 6.44D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84265790625 IErMin=14 ErrMin= 6.44D-07

ErrMax= 6.44D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.62D-10 BMatP= 1.39D-09

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

Coeff-Com: -0.345D-04 0.124D-02 0.996D-03-0.148D-03-0.204D-02-0.515D-02

Coeff-Com: 0.652D-02 0.193D-01 0.972D-03-0.569D-01-0.141D+00 0.305D-03

Coeff-Com: 0.599D+00 0.577D+00

Coeff: -0.345D-04 0.124D-02 0.996D-03-0.148D-03-0.204D-02-0.515D-02

Coeff: 0.652D-02 0.193D-01 0.972D-03-0.569D-01-0.141D+00 0.305D-03

Coeff: 0.599D+00 0.577D+00

Gap= 0.055 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.80D-08 MaxDP=2.40D-06 DE=-1.94D-09 OVMax= 1.41D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 1.86D-08 CP: 1.00D+00 1.40D+00 2.23D+00 2.71D+00 3.00D+00

CP: 3.00D+00 1.84D+00 2.21D+00 1.57D+00 1.82D+00

CP: 1.89D+00 1.43D+00 1.43D+00 8.82D-01

E= -1275.84265790654 Delta-E= -0.000000000290 Rises=F Damp=F

DIIS: error= 1.86D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.84265790654 IErMin=15 ErrMin= 1.86D-07

ErrMax= 1.86D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.27D-11 BMatP= 6.62D-10

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

Coeff-Com: -0.188D-04 0.263D-03 0.609D-03 0.496D-03 0.730D-03-0.305D-02

Coeff-Com: -0.985D-04 0.188D-02 0.109D-01 0.558D-02-0.355D-01-0.422D-01

Coeff-Com: -0.130D-01 0.135D+00 0.938D+00

Coeff: -0.188D-04 0.263D-03 0.609D-03 0.496D-03 0.730D-03-0.305D-02

Coeff: -0.985D-04 0.188D-02 0.109D-01 0.558D-02-0.355D-01-0.422D-01

Coeff: -0.130D-01 0.135D+00 0.938D+00

Gap= 0.055 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.58D-08 MaxDP=1.10D-06 DE=-2.90D-10 OVMax= 5.82D-06

Cycle 16 Pass 1 IDiag 1:

RMSU= 9.02D-09 CP: 1.00D+00 1.40D+00 2.23D+00 2.71D+00 3.00D+00

CP: 3.00D+00 1.84D+00 2.21D+00 1.57D+00 1.83D+00

CP: 1.91D+00 1.46D+00 1.48D+00 1.02D+00 1.18D+00

E= -1275.84265790659 Delta-E= -0.000000000051 Rises=F Damp=F

DIIS: error= 1.40D-07 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1275.84265790659 IErMin=16 ErrMin= 1.40D-07

ErrMax= 1.40D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.30D-11 BMatP= 4.27D-11

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

Coeff-Com: -0.773D-05-0.381D-04 0.306D-03 0.556D-03 0.987D-03-0.136D-02

Coeff-Com: -0.155D-02-0.267D-02 0.745D-02 0.157D-01 0.641D-02-0.245D-01

Coeff-Com: -0.121D+00-0.392D-01 0.544D+00 0.614D+00

Coeff: -0.773D-05-0.381D-04 0.306D-03 0.556D-03 0.987D-03-0.136D-02

Coeff: -0.155D-02-0.267D-02 0.745D-02 0.157D-01 0.641D-02-0.245D-01

Coeff: -0.121D+00-0.392D-01 0.544D+00 0.614D+00

Gap= 0.055 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.73D-08 MaxDP=8.76D-07 DE=-5.09D-11 OVMax= 1.27D-05

Cycle 17 Pass 1 IDiag 1:

RMSU= 3.78D-09 CP: 1.00D+00 1.40D+00 2.23D+00 2.71D+00 3.00D+00

CP: 3.00D+00 1.84D+00 2.21D+00 1.57D+00 1.83D+00

CP: 1.92D+00 1.46D+00 1.48D+00 1.04D+00 1.36D+00

CP: 1.15D+00

E= -1275.84265790663 Delta-E= -0.000000000032 Rises=F Damp=F

DIIS: error= 5.25D-08 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=17 EnMin= -1275.84265790663 IErMin=17 ErrMin= 5.25D-08

ErrMax= 5.25D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.02D-12 BMatP= 2.30D-11

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

Coeff-Com: 0.138D-05-0.522D-04-0.442D-04 0.345D-05 0.650D-04 0.215D-03

Coeff-Com: -0.876D-04-0.932D-03 0.348D-03 0.206D-02 0.650D-02 0.241D-03

Coeff-Com: -0.262D-01-0.351D-01-0.300D-01 0.158D+00 0.925D+00

Coeff: 0.138D-05-0.522D-04-0.442D-04 0.345D-05 0.650D-04 0.215D-03

Coeff: -0.876D-04-0.932D-03 0.348D-03 0.206D-02 0.650D-02 0.241D-03

Coeff: -0.262D-01-0.351D-01-0.300D-01 0.158D+00 0.925D+00

Gap= 0.055 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.47D-09 MaxDP=2.09D-07 DE=-3.18D-11 OVMax= 2.69D-06

Error on total polarization charges = 0.06482

SCF Done: E(UB3LYP) = -1275.84265791 A.U. after 17 cycles

NFock= 17 Conv=0.45D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0184 S= 1.0061

<L.S>= 0.000000000000E+00

KE= 1.320766263481D+03 PE=-8.572988692069D+03 EE= 3.215839207281D+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 2.0184, after 2.0002

Leave Link 502 at Tue Sep 17 14:13:02 2019, MaxMem= 2415919104 cpu: 1571.9

(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= 15315 LenP2D= 41258.

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 = 256

Leave Link 701 at Tue Sep 17 14:13:06 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 14:13:06 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 14:13:16 2019, MaxMem= 2415919104 cpu: 175.2

(Enter /home/blab/g09/l716.exe)

Dipole =-2.47801779D-13-3.69482223D-13-2.22044605D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.008922336 0.004378090 -0.000000000

2 7 0.003982846 -0.000445927 -0.000000000

3 6 0.007191678 0.000935632 -0.000000000

4 6 -0.002620677 0.001756859 0.000000000

5 6 -0.001927377 -0.001482162 0.000000000

6 7 -0.003174095 -0.002225641 0.000000000

7 6 0.001031153 0.000849660 -0.000000000

8 7 -0.002824336 -0.003586097 0.000000000

9 6 0.004245690 0.001330926 0.000000000

10 6 0.001397136 0.006192423 -0.000000000

11 6 -0.003355375 -0.000891413 -0.000000000

12 7 0.004037646 -0.002853748 -0.000000000

13 6 -0.001397136 -0.006192423 -0.000000000

14 6 0.003355375 0.000891413 -0.000000000

15 6 -0.001031153 -0.000849660 -0.000000000

16 7 0.002824336 0.003586097 -0.000000000

17 6 -0.004245690 -0.001330926 -0.000000000

18 7 0.003174095 0.002225641 -0.000000000

19 7 -0.003982846 0.000445927 0.000000000

20 6 -0.007191678 -0.000935632 0.000000000

21 6 0.002620677 -0.001756859 -0.000000000

22 6 0.001927377 0.001482162 0.000000000

23 6 0.008922336 -0.004378090 0.000000000

24 7 -0.004037646 0.002853748 -0.000000000

25 30 -0.000000000 0.000000000 0.000000000

26 6 0.000865161 0.000604098 -0.000000000

27 1 -0.000668081 0.000046100 -0.000000000

28 6 0.001353514 0.000835684 0.000000000

29 1 -0.000838205 0.001677011 -0.000000000

30 6 -0.001353514 -0.000835684 -0.000000000

31 1 0.000838205 -0.001677011 -0.000000000

32 6 -0.000865161 -0.000604098 -0.000000000

33 1 0.000668081 -0.000046100 -0.000000000

34 1 0.000380142 0.000357113 -0.000000000

35 1 -0.000792620 0.000513216 -0.000578137

36 1 -0.000792620 0.000513216 0.000578137

37 1 -0.000379297 -0.000806671 -0.000648794

38 1 -0.000379297 -0.000806671 0.000648794

39 1 0.000305939 0.000426953 -0.000000000

40 1 0.000379297 0.000806671 -0.000648794

41 1 0.000379297 0.000806671 0.000648794

42 1 -0.000305939 -0.000426953 -0.000000000

43 1 0.000792620 -0.000513216 -0.000578137

44 1 0.000792620 -0.000513216 0.000578137

45 1 -0.000380142 -0.000357113 0.000000000

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

Cartesian Forces: Max 0.008922336 RMS 0.002213035

Leave Link 716 at Tue Sep 17 14:13:16 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 0.007215311 RMS 0.001306626

Search for a local minimum.

Step number 13 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 12 13

DE= -1.25D-04 DEPred=-1.91D-04 R= 6.54D-01

TightC=F SS= 1.41D+00 RLast= 1.06D-01 DXNew= 4.4366D-01 3.1676D-01

Trust test= 6.54D-01 RLast= 1.06D-01 DXMaxT set to 3.17D-01

ITU= 1 1 1 -1 0 1 -1 1 1 1 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01331

Eigenvalues --- 0.01332 0.01349 0.01350 0.01601 0.01622

Eigenvalues --- 0.01628 0.01640 0.01772 0.01794 0.01806

Eigenvalues --- 0.01826 0.01887 0.01910 0.01937 0.01950

Eigenvalues --- 0.01995 0.02000 0.02044 0.02047 0.02070

Eigenvalues --- 0.02086 0.02102 0.02109 0.02115 0.02205

Eigenvalues --- 0.02312 0.02317 0.02351 0.02372 0.04263

Eigenvalues --- 0.07191 0.07191 0.07203 0.07203 0.07246

Eigenvalues --- 0.07287 0.07369 0.07770 0.12116 0.14444

Eigenvalues --- 0.14495 0.14501 0.15799 0.15957 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16019

Eigenvalues --- 0.16071 0.16369 0.16762 0.17270 0.19920

Eigenvalues --- 0.22056 0.22092 0.23035 0.23840 0.23857

Eigenvalues --- 0.23957 0.24905 0.24977 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25008

Eigenvalues --- 0.26451 0.29763 0.30936 0.31218 0.32793

Eigenvalues --- 0.33177 0.33191 0.33282 0.33282 0.33314

Eigenvalues --- 0.33711 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33724 0.33943 0.34402 0.34437

Eigenvalues --- 0.34437 0.34441 0.34800 0.35552 0.35578

Eigenvalues --- 0.35641 0.35682 0.35682 0.35864 0.36530

Eigenvalues --- 0.39074 0.40559 0.41648 0.41840 0.43239

Eigenvalues --- 0.47739 0.48945 0.48996 0.50223 0.51357

Eigenvalues --- 0.51362 0.51580 0.53056 0.54013 0.54024

Eigenvalues --- 0.54715 0.56321 0.56330 0.56539

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 0.20528 0.61716 0.33709 -0.15952

Cosine: 0.996 > 0.710

Length: 1.026

GDIIS step was calculated using 4 of the last 13 vectors.

Iteration 1 RMS(Cart)= 0.01435317 RMS(Int)= 0.00003007

Iteration 2 RMS(Cart)= 0.00007868 RMS(Int)= 0.00000747

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000747

ITry= 1 IFail=0 DXMaxC= 5.00D-02 DCOld= 1.00D+10 DXMaxT= 3.17D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 3.27D-09 for atom 27.

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

(Linear) (Quad) (Total)

R1 2.55804 0.00519 0.02284 -0.00083 0.02200 2.58004

R2 2.74030 -0.00116 -0.00900 -0.00134 -0.01035 2.72995

R3 2.60791 -0.00722 -0.02128 0.00353 -0.01775 2.59016

R4 2.57516 -0.00063 -0.01111 0.00040 -0.01071 2.56445

R5 3.80146 -0.00149 -0.00645 -0.00067 -0.00713 3.79433

R6 2.76128 0.00182 0.00755 0.00126 0.00882 2.77011

R7 2.58104 -0.00117 -0.00168 0.00471 0.00304 2.58408

R8 2.59845 0.00025 0.00258 -0.00242 0.00017 2.59862

R9 2.81879 -0.00199 -0.00412 -0.00434 -0.00846 2.81034

R10 2.04190 0.00055 0.00115 0.00004 0.00119 2.04309

R11 2.48674 0.00289 0.01017 -0.00509 0.00510 2.49184

R12 2.59891 -0.00172 -0.01511 0.00181 -0.01330 2.58561

R13 2.79907 -0.00056 -0.00035 0.00420 0.00386 2.80293

R14 2.55814 0.00427 0.02043 -0.00157 0.01884 2.57699

R15 3.77795 -0.00082 -0.00126 -0.00060 -0.00187 3.77608

R16 2.85896 -0.00370 -0.02152 0.00710 -0.01442 2.84454

R17 2.49626 -0.00262 -0.00726 -0.00708 -0.01434 2.48193

R18 2.54388 0.00323 0.00800 -0.00551 0.00251 2.54639

R19 2.80464 0.00076 0.00402 -0.00215 0.00187 2.80651

R20 2.04773 -0.00187 -0.00400 -0.00253 -0.00653 2.04121

R21 2.49626 -0.00262 -0.00726 -0.00708 -0.01434 2.48193

R22 2.54388 0.00323 0.00800 -0.00551 0.00251 2.54639

R23 2.85896 -0.00370 -0.02152 0.00710 -0.01442 2.84454

R24 2.80464 0.00076 0.00402 -0.00215 0.00187 2.80651

R25 2.79907 -0.00056 -0.00035 0.00420 0.00386 2.80293

R26 2.04773 -0.00187 -0.00400 -0.00253 -0.00653 2.04121

R27 2.59891 -0.00172 -0.01511 0.00181 -0.01330 2.58561

R28 2.48674 0.00289 0.01017 -0.00509 0.00510 2.49184

R29 2.55814 0.00427 0.02043 -0.00157 0.01884 2.57699

R30 3.77795 -0.00082 -0.00126 -0.00060 -0.00187 3.77608

R31 2.58104 -0.00117 -0.00168 0.00471 0.00304 2.58408

R32 2.57516 -0.00063 -0.01111 0.00040 -0.01071 2.56445

R33 2.55804 0.00519 0.02284 -0.00083 0.02200 2.58004

R34 3.80146 -0.00149 -0.00645 -0.00067 -0.00713 3.79433

R35 2.76128 0.00182 0.00755 0.00126 0.00882 2.77011

R36 2.59845 0.00025 0.00258 -0.00242 0.00017 2.59862

R37 2.81879 -0.00199 -0.00412 -0.00434 -0.00846 2.81034

R38 2.74030 -0.00116 -0.00900 -0.00134 -0.01035 2.72995

R39 2.04190 0.00055 0.00115 0.00004 0.00119 2.04309

R40 2.60791 -0.00722 -0.02128 0.00353 -0.01775 2.59016

R41 2.06371 -0.00052 -0.00083 -0.00146 -0.00228 2.06143

R42 2.07220 -0.00101 -0.00163 -0.00305 -0.00467 2.06752

R43 2.07220 -0.00101 -0.00163 -0.00305 -0.00467 2.06752

R44 2.07210 -0.00105 -0.00227 -0.00272 -0.00498 2.06712

R45 2.07210 -0.00105 -0.00227 -0.00272 -0.00498 2.06712

R46 2.06220 -0.00014 -0.00014 -0.00114 -0.00128 2.06093

R47 2.07210 -0.00105 -0.00227 -0.00272 -0.00498 2.06712

R48 2.07210 -0.00105 -0.00227 -0.00272 -0.00498 2.06712

R49 2.06220 -0.00014 -0.00014 -0.00114 -0.00128 2.06093

R50 2.07220 -0.00101 -0.00163 -0.00305 -0.00467 2.06752

R51 2.07220 -0.00101 -0.00163 -0.00305 -0.00467 2.06752

R52 2.06371 -0.00052 -0.00083 -0.00146 -0.00228 2.06143

A1 1.89436 -0.00006 0.00035 -0.00090 -0.00057 1.89379

A2 2.20298 0.00149 0.00123 0.00298 0.00421 2.20719

A3 2.18585 -0.00143 -0.00158 -0.00208 -0.00364 2.18221

A4 1.90057 0.00128 0.00271 0.00413 0.00685 1.90742

A5 2.19936 -0.00069 -0.00881 0.00224 -0.00656 2.19280

A6 2.18325 -0.00059 0.00610 -0.00637 -0.00029 2.18297

A7 1.90632 -0.00316 -0.00731 -0.00633 -0.01362 1.89269

A8 2.21497 0.00124 0.00414 0.00654 0.01067 2.22565

A9 2.16190 0.00192 0.00316 -0.00021 0.00295 2.16485

A10 1.84059 0.00366 0.00976 0.00466 0.01442 1.85501

A11 2.18529 -0.00244 -0.00653 -0.00582 -0.01235 2.17294

A12 2.25731 -0.00122 -0.00323 0.00116 -0.00207 2.25524

A13 1.88294 -0.00172 -0.00550 -0.00156 -0.00707 1.87587

A14 2.18143 0.00048 0.00203 -0.00059 0.00144 2.18287

A15 2.21882 0.00124 0.00348 0.00215 0.00563 2.22445

A16 2.17915 -0.00120 -0.01075 -0.00483 -0.01555 2.16360

A17 2.22982 0.00001 0.00047 0.00401 0.00450 2.23431

A18 2.16502 0.00181 0.00271 0.00080 0.00350 2.16853

A19 1.88835 -0.00183 -0.00319 -0.00481 -0.00800 1.88035

A20 1.91390 0.00054 -0.00172 0.00354 0.00182 1.91573

A21 2.18455 -0.00002 0.00739 -0.00302 0.00437 2.18892

A22 2.18473 -0.00052 -0.00567 -0.00052 -0.00619 2.17853

A23 1.88109 0.00091 0.00472 -0.00159 0.00311 1.88420

A24 2.25105 0.00061 -0.00612 0.00915 0.00303 2.25408

A25 2.15105 -0.00153 0.00140 -0.00756 -0.00614 2.14491

A26 1.86347 -0.00224 -0.00649 -0.00158 -0.00807 1.85540

A27 2.14797 0.00130 0.00944 -0.00489 0.00455 2.15251

A28 2.27175 0.00095 -0.00294 0.00647 0.00353 2.27527

A29 1.87797 0.00262 0.00669 0.00444 0.01114 1.88911

A30 2.16657 -0.00121 0.00004 -0.00418 -0.00414 2.16242

A31 2.23865 -0.00141 -0.00673 -0.00026 -0.00699 2.23166

A32 2.16130 -0.00034 0.01201 -0.01018 0.00181 2.16310

A33 1.86347 -0.00224 -0.00649 -0.00158 -0.00807 1.85540

A34 2.27175 0.00095 -0.00294 0.00647 0.00353 2.27527

A35 2.14797 0.00130 0.00944 -0.00489 0.00455 2.15251

A36 1.87797 0.00262 0.00669 0.00444 0.01114 1.88911

A37 2.23865 -0.00141 -0.00673 -0.00026 -0.00699 2.23166

A38 2.16657 -0.00121 0.00004 -0.00418 -0.00414 2.16242

A39 1.88835 -0.00183 -0.00319 -0.00481 -0.00800 1.88035

A40 2.16502 0.00181 0.00271 0.00080 0.00350 2.16853

A41 2.22982 0.00001 0.00047 0.00401 0.00450 2.23431

A42 1.91390 0.00054 -0.00172 0.00354 0.00182 1.91573

A43 2.18455 -0.00002 0.00739 -0.00302 0.00437 2.18892

A44 2.18473 -0.00052 -0.00567 -0.00052 -0.00619 2.17853

A45 2.15105 -0.00153 0.00140 -0.00756 -0.00614 2.14491

A46 2.25105 0.00061 -0.00612 0.00915 0.00303 2.25408

A47 1.88109 0.00091 0.00472 -0.00159 0.00311 1.88420

A48 2.17915 -0.00120 -0.01075 -0.00483 -0.01555 2.16360

A49 1.90057 0.00128 0.00271 0.00413 0.00685 1.90742

A50 2.18325 -0.00059 0.00610 -0.00637 -0.00029 2.18297

A51 2.19936 -0.00069 -0.00881 0.00224 -0.00656 2.19280

A52 2.21497 0.00124 0.00414 0.00654 0.01067 2.22565

A53 2.16190 0.00192 0.00316 -0.00021 0.00295 2.16485

A54 1.90632 -0.00316 -0.00731 -0.00633 -0.01362 1.89269

A55 1.84059 0.00366 0.00976 0.00466 0.01442 1.85501

A56 2.18529 -0.00244 -0.00653 -0.00582 -0.01235 2.17294

A57 2.25731 -0.00122 -0.00323 0.00116 -0.00207 2.25524

A58 1.88294 -0.00172 -0.00550 -0.00156 -0.00707 1.87587

A59 2.21882 0.00124 0.00348 0.00215 0.00563 2.22445

A60 2.18143 0.00048 0.00203 -0.00059 0.00144 2.18287

A61 1.89436 -0.00006 0.00035 -0.00090 -0.00057 1.89379

A62 2.20298 0.00149 0.00123 0.00298 0.00421 2.20719

A63 2.18585 -0.00143 -0.00158 -0.00208 -0.00364 2.18221

A64 2.16130 -0.00034 0.01201 -0.01018 0.00181 2.16310

A65 1.57462 0.00055 -0.00736 0.00368 -0.00370 1.57092

A66 1.56697 -0.00055 0.00736 -0.00368 0.00370 1.57067

A67 1.56697 -0.00055 0.00736 -0.00368 0.00370 1.57067

A68 1.57462 0.00055 -0.00736 0.00368 -0.00370 1.57092

A69 1.94140 0.00007 -0.00007 0.00259 0.00254 1.94394

A70 1.94340 -0.00043 -0.00301 -0.00026 -0.00328 1.94012

A71 1.94340 -0.00043 -0.00301 -0.00026 -0.00328 1.94012

A72 1.88905 0.00015 0.00041 0.00047 0.00089 1.88993

A73 1.88905 0.00015 0.00041 0.00047 0.00089 1.88993

A74 1.85418 0.00054 0.00566 -0.00323 0.00241 1.85660

A75 1.93685 -0.00042 -0.00300 -0.00017 -0.00316 1.93369

A76 1.93685 -0.00042 -0.00300 -0.00017 -0.00316 1.93369

A77 1.94169 0.00084 0.00134 0.00496 0.00630 1.94799

A78 1.85337 0.00039 0.00684 -0.00514 0.00169 1.85506

A79 1.89613 -0.00020 -0.00095 0.00003 -0.00092 1.89522

A80 1.89613 -0.00020 -0.00095 0.00003 -0.00092 1.89522

A81 1.93685 -0.00042 -0.00300 -0.00017 -0.00316 1.93369

A82 1.93685 -0.00042 -0.00300 -0.00017 -0.00316 1.93369

A83 1.94169 0.00084 0.00134 0.00496 0.00630 1.94799

A84 1.85337 0.00039 0.00684 -0.00514 0.00169 1.85506

A85 1.89613 -0.00020 -0.00095 0.00003 -0.00092 1.89522

A86 1.89613 -0.00020 -0.00095 0.00003 -0.00092 1.89522

A87 1.94340 -0.00043 -0.00301 -0.00026 -0.00328 1.94012

A88 1.94340 -0.00043 -0.00301 -0.00026 -0.00328 1.94012

A89 1.94140 0.00007 -0.00007 0.00259 0.00254 1.94394

A90 1.85418 0.00054 0.00566 -0.00323 0.00241 1.85660

A91 1.88905 0.00015 0.00041 0.00047 0.00089 1.88993

A92 1.88905 0.00015 0.00041 0.00047 0.00089 1.88993

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

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D31 -1.03293 -0.00006 -0.00157 0.00220 0.00062 -1.03231

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D33 -2.10866 0.00006 0.00157 -0.00220 -0.00062 -2.10928

D34 2.10866 -0.00006 -0.00157 0.00220 0.00062 2.10928

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D63 1.02820 -0.00002 0.00235 -0.00331 -0.00095 1.02725

D64 -1.02820 0.00002 -0.00235 0.00331 0.00095 -1.02725

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D66 -2.11339 -0.00002 0.00235 -0.00331 -0.00095 -2.11434

D67 2.11339 0.00002 -0.00235 0.00331 0.00095 2.11434

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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

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D114 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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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

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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 1.03293 0.00006 0.00157 -0.00220 -0.00062 1.03231

D126 -1.03293 -0.00006 -0.00157 0.00220 0.00062 -1.03231

D127 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D128 -2.10866 0.00006 0.00157 -0.00220 -0.00062 -2.10928

D129 2.10866 -0.00006 -0.00157 0.00220 0.00062 2.10928

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

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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 0.007215 0.000450 NO

RMS Force 0.001307 0.000300 NO

Maximum Displacement 0.050027 0.001800 NO

RMS Displacement 0.014337 0.001200 NO

Predicted change in Energy=-8.568121D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:13:16 2019, MaxMem= 2415919104 cpu: 1.4

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.073542 -2.188741 0.000000

2 7 0 -0.747541 -1.863527 0.000000

3 6 0 -0.007101 -3.000771 0.000000

4 6 0 -0.919415 -4.148151 0.000000

5 6 0 -2.192563 -3.628458 0.000000

6 7 0 1.356208 -3.106933 0.000000

7 6 0 2.175590 -2.073788 0.000000

8 7 0 1.854657 -0.743711 0.000000

9 6 0 2.994059 0.005550 0.000000

10 6 0 4.168574 -0.935909 0.000000

11 6 0 3.654907 -2.181654 0.000000

12 7 0 -3.127251 -1.312159 0.000000

13 6 0 -4.168574 0.935909 0.000000

14 6 0 -3.654907 2.181654 0.000000

15 6 0 -2.175590 2.073788 0.000000

16 7 0 -1.854657 0.743711 0.000000

17 6 0 -2.994059 -0.005550 0.000000

18 7 0 -1.356208 3.106933 0.000000

19 7 0 0.747541 1.863527 0.000000

20 6 0 0.007101 3.000771 0.000000

21 6 0 0.919415 4.148151 0.000000

22 6 0 2.192563 3.628458 0.000000

23 6 0 2.073542 2.188741 0.000000

24 7 0 3.127251 1.312159 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.484351 -5.570256 0.000000

27 1 0 -3.125614 -4.174639 0.000000

28 6 0 5.581384 -0.478075 0.000000

29 1 0 4.190530 -3.119659 0.000000

30 6 0 -5.581384 0.478075 0.000000

31 1 0 -4.190530 3.119659 0.000000

32 6 0 0.484351 5.570256 0.000000

33 1 0 3.125614 4.174639 0.000000

34 1 0 -1.339372 -6.247691 0.000000

35 1 0 0.131549 -5.794853 0.875926

36 1 0 0.131549 -5.794853 -0.875926

37 1 0 5.787737 0.144746 0.875252

38 1 0 5.787737 0.144746 -0.875252

39 1 0 6.276068 -1.318798 0.000000

40 1 0 -5.787737 -0.144746 0.875252

41 1 0 -5.787737 -0.144746 -0.875252

42 1 0 -6.276068 1.318798 0.000000

43 1 0 -0.131549 5.794853 0.875926

44 1 0 -0.131549 5.794853 -0.875926

45 1 0 1.339372 6.247691 0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.365300 0.000000

3 C 2.220264 1.357047 0.000000

4 C 2.274049 2.291080 1.465878 0.000000

5 C 1.444628 2.281024 2.273815 1.375131 0.000000

6 N 3.550530 2.443730 1.367436 2.502518 3.586888

7 C 4.250687 2.930683 2.371379 3.725861 4.636567

8 N 4.185554 2.832917 2.925827 4.391548 4.970086

9 C 5.522273 4.182466 4.247932 5.706883 6.333013

10 C 6.366600 5.002865 4.658317 6.017153 6.907523

11 C 5.728454 4.413927 3.752500 4.979110 6.023798

12 N 1.370655 2.442749 3.547780 3.594077 2.497775

13 C 3.761993 4.420442 5.728465 6.033631 4.973738

14 C 4.647694 4.981593 6.337509 6.895603 5.991314

15 C 4.263750 4.188290 5.518469 6.347480 5.702271

16 N 2.940609 2.832560 4.175477 4.980461 4.385207

17 C 2.369319 2.915291 4.230043 4.633065 3.710506

18 N 5.344037 5.007589 6.254930 7.268221 6.787119

19 N 4.937549 4.015744 4.922488 6.238511 6.229455

20 C 5.591075 4.922488 6.001560 7.208712 6.984641

21 C 7.008138 6.238511 7.208712 8.497643 8.376160

22 C 7.213838 6.229455 6.984641 8.376160 8.478924

23 C 6.029980 4.937549 5.591075 7.008138 7.213838

24 N 6.269334 5.009889 5.331560 6.796359 7.260173

25 Zn 3.014990 2.007872 3.000780 4.248822 4.239462

26 C 3.736332 3.716061 2.613430 1.487166 2.586227

27 H 2.247364 3.316093 3.332130 2.206358 1.081156

28 C 7.843742 6.478794 6.131489 7.465243 8.388037

29 H 6.332868 5.095333 4.199314 5.212422 6.403339

30 C 4.406457 5.371140 6.570770 6.567795 5.324259

31 H 5.714958 6.056923 7.413552 7.970023 7.037682

32 C 8.169752 7.535163 8.585106 9.819267 9.580303

33 H 8.217289 7.173617 7.829458 9.253708 9.443057

34 H 4.124813 4.423930 3.509620 2.141128 2.754690

35 H 4.316679 4.122544 2.931444 2.140888 3.295756

36 H 4.316679 4.122544 2.931444 2.140888 3.295756

37 H 8.246875 6.892683 6.651353 8.011300 8.870644

38 H 8.246875 6.892683 6.651353 8.011300 8.870644

39 H 8.394808 7.044701 6.504402 7.731767 8.777940

40 H 4.328882 5.396652 6.506819 6.363480 5.082085

41 H 4.328882 5.396652 6.506819 6.363480 5.082085

42 H 5.473943 6.379013 7.613056 7.653840 6.414854

43 H 8.262951 7.732883 8.840008 10.012558 9.685753

44 H 8.262951 7.732883 8.840008 10.012558 9.685753

45 H 9.100624 8.375384 9.345964 10.638405 10.488702

6 7 8 9 10

6 N 0.000000

7 C 1.318626 0.000000

8 N 2.415217 1.368248 0.000000

9 C 3.517117 2.234623 1.363682 0.000000

10 C 3.552850 2.294941 2.321886 1.505268 0.000000

11 C 2.477934 1.483245 2.304036 2.284859 1.347491

12 N 4.829349 5.357256 5.014233 6.261532 7.305519

13 C 6.846005 7.021872 6.253033 7.222802 8.544690

14 C 7.285631 7.218274 6.238032 6.996011 8.421760

15 C 6.270045 6.011252 4.917437 5.568022 7.021872

16 N 5.013692 4.917437 3.996427 4.904582 6.253033

17 C 5.342602 5.568022 4.904582 5.988128 7.222802

18 N 6.780069 6.270045 5.013692 5.342602 6.846005

19 N 5.007589 4.188290 2.832560 2.915291 4.420442

20 C 6.254930 5.518469 4.175477 4.230043 5.728465

21 C 7.268221 6.347480 4.980461 4.633065 6.033631

22 C 6.787119 5.702271 4.385207 3.710506 4.973738

23 C 5.344037 4.263750 2.940609 2.369319 3.761993

24 N 4.760774 3.517143 2.417870 1.313380 2.477532

25 Zn 3.390035 3.005626 1.998213 2.994064 4.272345

26 C 3.074999 4.393242 5.363441 6.571830 6.567105

27 H 4.607247 5.702310 6.047674 7.411098 7.980886

28 C 4.976244 3.761082 3.736183 2.632138 1.485142

29 H 2.834351 2.270205 3.331882 3.346413 2.183860

30 C 7.809128 8.165945 7.535746 8.588452 9.851956

31 H 8.338870 8.215800 7.174253 7.830453 9.290977

32 C 8.720880 7.828901 6.460953 6.104472 7.476877

33 H 7.493470 6.320236 5.079911 4.171164 5.215886

34 H 4.138902 5.456777 6.363616 7.607999 7.651960

35 H 3.080901 4.334937 5.408363 6.527319 6.377629

36 H 3.080901 4.334937 5.408363 6.527319 6.377629

37 H 5.565782 4.328460 4.126081 2.930884 2.134379

38 H 5.565782 4.328460 4.126081 2.930884 2.134379

39 H 5.234735 4.169404 4.458655 3.539136 2.141993

40 H 7.783095 8.240257 7.715634 8.826584 10.025973

41 H 7.783095 8.240257 7.715634 8.826584 10.025973

42 H 8.822626 9.107148 8.388243 9.362685 10.685235

43 H 9.067661 8.246554 6.889490 6.637221 8.035015

44 H 9.067661 8.246554 6.889490 6.637221 8.035015

45 H 9.354639 8.363389 7.010365 6.457732 7.720654

11 12 13 14 15

11 C 0.000000

12 N 6.837666 0.000000

13 C 8.421760 2.477532 0.000000

14 C 8.513039 3.533433 1.347491 0.000000

15 C 7.218274 3.517143 2.294941 1.483245 0.000000

16 N 6.238032 2.417870 2.321886 2.304036 1.368248

17 C 6.996011 1.313380 1.505268 2.284859 2.234623

18 N 7.285631 4.760774 3.552850 2.477934 1.318626

19 N 4.981593 5.009889 5.002865 4.413927 2.930683

20 C 6.337509 5.331560 4.658317 3.752500 2.371379

21 C 6.895603 6.796359 6.017153 4.979110 3.725861

22 C 5.991314 7.260173 6.907523 6.023798 4.636567

23 C 4.647694 6.269334 6.366600 5.728454 4.250687

24 N 3.533433 6.782760 7.305519 6.837666 5.357256

25 Zn 4.256519 3.391380 4.272345 4.256519 3.005626

26 C 5.349400 5.011617 7.476877 8.375233 7.828901

27 H 7.067351 2.862480 5.215886 6.378292 6.320236

28 C 2.571671 8.748487 9.851956 9.611620 8.165945

29 H 1.080161 7.537703 9.290977 9.468622 8.215800

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32 C 8.375233 7.772471 6.567105 5.349400 4.393242

33 H 6.378292 8.318850 7.980886 7.067351 5.702310

34 H 6.440146 5.249379 7.720654 8.741599 8.363389

35 H 5.122159 5.610844 8.035015 8.872945 8.246554

36 H 5.122159 5.610844 8.035015 8.872945 8.246554

37 H 3.275235 9.075552 10.025973 9.699411 8.240257

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39 H 2.759530 9.403321 10.685235 10.529835 9.107148

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42 H 10.529835 4.103290 2.141993 2.759530 4.169404

43 H 8.872945 7.762158 6.377629 5.122159 4.334937

44 H 8.872945 7.762158 6.377629 5.122159 4.334937

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16 17 18 19 20

16 N 0.000000

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18 N 2.415217 3.517117 0.000000

19 N 2.832917 4.182466 2.443730 0.000000

20 C 2.925827 4.247932 1.367436 1.357047 0.000000

21 C 4.391548 5.706883 2.502518 2.291080 1.465878

22 C 4.970086 6.333013 3.586888 2.281024 2.273815

23 C 4.185554 5.522273 3.550530 1.365300 2.220264

24 N 5.014233 6.261532 4.829349 2.442749 3.547780

25 Zn 1.998213 2.994064 3.390035 2.007872 3.000780

26 C 6.460953 6.104472 8.720880 7.535163 8.585106

27 H 5.079911 4.171164 7.493470 7.173617 7.829458

28 C 7.535746 8.588452 7.809128 5.371140 6.570770

29 H 7.174253 7.830453 8.338870 6.056923 7.413552

30 C 3.736183 2.632138 4.976244 6.478794 6.131489

31 H 3.331882 3.346413 2.834351 5.095333 4.199314

32 C 5.363441 6.571830 3.074999 3.716061 2.613430

33 H 6.047674 7.411098 4.607247 3.316093 3.332130

34 H 7.010365 6.457732 9.354639 8.375384 9.345964

35 H 6.889490 6.637221 9.067661 7.732883 8.840008

36 H 6.889490 6.637221 9.067661 7.732883 8.840008

37 H 7.715634 8.826584 7.783095 5.396652 6.506819

38 H 7.715634 8.826584 7.783095 5.396652 6.506819

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40 H 4.126081 2.930884 5.565782 6.892683 6.651353

41 H 4.126081 2.930884 5.565782 6.892683 6.651353

42 H 4.458655 3.539136 5.234735 7.044701 6.504402

43 H 5.408363 6.527319 3.080901 4.122544 2.931444

44 H 5.408363 6.527319 3.080901 4.122544 2.931444

45 H 6.363616 7.607999 4.138902 4.423930 3.509620

21 22 23 24 25

21 C 0.000000

22 C 1.375131 0.000000

23 C 2.274049 1.444628 0.000000

24 N 3.594077 2.497775 1.370655 0.000000

25 Zn 4.248822 4.239462 3.014990 3.391380 0.000000

26 C 9.819267 9.580303 8.169752 7.772471 5.591274

27 H 9.253708 9.443057 8.217289 8.318850 5.215081

28 C 6.567795 5.324259 4.406457 3.037715 5.601822

29 H 7.970023 7.037682 5.714958 4.557585 5.224253

30 C 7.465243 8.388037 7.843742 8.748487 5.601822

31 H 5.212422 6.403339 6.332868 7.537703 5.224253

32 C 1.487166 2.586227 3.736332 5.011617 5.591274

33 H 2.206358 1.081156 2.247364 2.862480 5.215081

34 H 10.638405 10.488702 9.100624 8.780777 6.389645

35 H 10.012558 9.685753 8.262951 7.762158 5.862156

36 H 10.012558 9.685753 8.262951 7.762158 5.862156

37 H 6.363480 5.082085 4.328882 3.034321 5.855332

38 H 6.363480 5.082085 4.328882 3.034321 5.855332

39 H 7.653840 6.414854 5.473943 4.103290 6.413132

40 H 8.011300 8.870644 8.246875 9.075552 5.855332

41 H 8.011300 8.870644 8.246875 9.075552 5.855332

42 H 7.731767 8.777940 8.394808 9.403321 6.413132

43 H 2.140888 3.295756 4.316679 5.610844 5.862156

44 H 2.140888 3.295756 4.316679 5.610844 5.862156

45 H 2.141128 2.754690 4.124813 5.249379 6.389645

26 27 28 29 30

26 C 0.000000

27 H 2.987310 0.000000

28 C 7.919813 9.459197 0.000000

29 H 5.278251 7.391816 2.985371 0.000000

30 C 7.909619 5.261042 11.203644 10.413165 0.000000

31 H 9.447243 7.371624 10.413165 10.448506 2.985371

32 C 11.182549 10.392056 7.909619 9.447243 7.919813

33 H 10.392056 10.430163 5.261042 7.371624 9.459197

34 H 1.090862 2.736458 9.010290 6.353298 7.951767

35 H 1.094086 3.741851 7.663947 4.939559 8.529624

36 H 1.094086 3.741851 7.663947 4.939559 8.529624

37 H 8.530322 9.943389 1.093871 3.738112 11.407633

38 H 8.530322 9.943389 1.093871 3.738112 11.407633

39 H 7.986123 9.825856 1.090596 2.755462 11.992828

40 H 7.637285 4.908462 11.407633 10.449019 1.093871

41 H 7.637285 4.908462 11.407633 10.449019 1.093871

42 H 9.000170 6.332709 11.992828 11.368799 1.090596

43 H 11.404272 10.446169 8.529624 9.945660 7.663947

44 H 11.404272 10.446169 8.529624 9.945660 7.663947

45 H 11.957836 11.338477 7.951767 9.791647 9.010290

31 32 33 34 35

31 H 0.000000

32 C 5.278251 0.000000

33 H 7.391816 2.987310 0.000000

34 H 9.791647 11.957836 11.338477 0.000000

35 H 9.945660 11.404272 10.446169 1.770852 0.000000

36 H 9.945660 11.404272 10.446169 1.770852 1.751853

37 H 10.449019 7.637285 4.908462 9.613792 8.201909

38 H 10.449019 7.637285 4.908462 9.613792 8.386771

39 H 11.368799 9.000170 6.332709 9.071323 7.652283

40 H 3.738112 8.530322 9.943389 7.602628 8.183010

41 H 3.738112 8.530322 9.943389 7.602628 8.368290

42 H 2.755462 7.986123 9.825856 9.034529 9.613992

43 H 4.939559 1.094086 3.741851 12.134618 11.592692

44 H 4.939559 1.094086 3.741851 12.134618 11.724312

45 H 6.353298 1.090862 2.736458 12.779289 12.134618

36 37 38 39 40

36 H 0.000000

37 H 8.386771 0.000000

38 H 8.201909 1.750504 0.000000

39 H 7.652283 1.773836 1.773836 0.000000

40 H 8.368290 11.579093 11.710665 12.152360 0.000000

41 H 8.183010 11.710665 11.579093 12.152360 1.750504

42 H 9.613992 12.152360 12.152360 12.826263 1.773836

43 H 11.724312 8.183010 8.368290 9.613992 8.201909

44 H 11.592692 8.368290 8.183010 9.613992 8.386771

45 H 12.134618 7.602628 7.602628 9.034529 9.613792

41 42 43 44 45

41 H 0.000000

42 H 1.773836 0.000000

43 H 8.386771 7.652283 0.000000

44 H 8.201909 7.652283 1.751853 0.000000

45 H 9.613792 9.071323 1.770852 1.770852 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=0 Diff= 1.07D+00

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 2.803243 -1.109951 0.000000

2 7 0 2.007872 -0.000254 0.000000

3 6 0 2.787831 1.110260 0.000000

4 6 0 4.192333 0.690529 0.000000

5 6 0 4.183825 -0.684575 0.000000

6 7 0 2.378959 2.415137 0.000000

7 6 0 1.115074 2.791128 0.000000

8 7 0 0.000000 1.998213 0.000000

9 6 0 -1.119504 2.776892 0.000000

10 6 0 -0.682821 4.217427 0.000000

11 6 0 0.664606 4.204314 0.000000

12 7 0 2.381815 -2.414211 0.000000

13 6 0 0.682821 -4.217427 0.000000

14 6 0 -0.664606 -4.204314 0.000000

15 6 0 -1.115074 -2.791128 0.000000

16 7 0 -0.000000 -1.998213 0.000000

17 6 0 1.119504 -2.776892 0.000000

18 7 0 -2.378959 -2.415137 0.000000

19 7 0 -2.007872 0.000254 0.000000

20 6 0 -2.787831 -1.110260 0.000000

21 6 0 -4.192333 -0.690529 0.000000

22 6 0 -4.183825 0.684575 0.000000

23 6 0 -2.803243 1.109951 0.000000

24 7 0 -2.381815 2.414211 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 5.350344 1.623628 0.000000

27 1 0 5.038038 -1.347312 0.000000

28 6 0 -1.633594 5.358337 0.000000

29 1 0 1.335870 5.050571 0.000000

30 6 0 1.633594 -5.358337 0.000000

31 1 0 -1.335870 -5.050571 0.000000

32 6 0 -5.350344 -1.623628 0.000000

33 1 0 -5.038038 1.347312 0.000000

34 1 0 6.297339 1.082167 0.000000

35 1 0 5.329575 2.278872 0.875926

36 1 0 5.329575 2.278872 -0.875926

37 1 0 -2.288473 5.318058 0.875252

38 1 0 -2.288473 5.318058 -0.875252

39 1 0 -1.111824 6.316020 0.000000

40 1 0 2.288473 -5.318058 0.875252

41 1 0 2.288473 -5.318058 -0.875252

42 1 0 1.111824 -6.316020 0.000000

43 1 0 -5.329575 -2.278872 0.875926

44 1 0 -5.329575 -2.278872 -0.875926

45 1 0 -6.297339 -1.082167 0.000000

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

Rotational constants (GHZ): 0.1832307 0.1820745 0.0915298

Leave Link 202 at Tue Sep 17 14:13:16 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 101 beta electrons

nuclear repulsion energy 2763.1343651094 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= -0.1143013580 Hartrees.

Nuclear repulsion after empirical dispersion term = 2763.0200637514 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 = 3490

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.37D-07

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 136

GePol: Fraction of low-weight points (<1% of avg) = 3.90%

GePol: Cavity surface area = 381.824 Ang\*\*2

GePol: Cavity volume = 379.153 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0107068854 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2763.0093568660 Hartrees.

Leave Link 301 at Tue Sep 17 14:13:16 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= 15339 LenP2D= 41300.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.83D-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 14:13:17 2019, MaxMem= 2415919104 cpu: 12.1

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:13:17 2019, MaxMem= 2415919104 cpu: 1.2

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= -0.000000 -0.000000 -0.000000

Rot= 0.925268 -0.000000 -0.000000 0.379313 Ang= 44.58 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 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0184 S= 1.0061

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= -1276.15085858190

Leave Link 401 at Tue Sep 17 14:13:19 2019, MaxMem= 2415919104 cpu: 38.6

(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 6.88D-15 for 3489.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.17D-15 for 2323 1259.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.11D-15 for 3489.

Iteration 1 A^-1\*A deviation from orthogonality is 5.04D-12 for 1766 1724.

E= -1275.84131601255

DIIS: error= 9.61D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.84131601255 IErMin= 1 ErrMin= 9.61D-04

ErrMax= 9.61D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.70D-03 BMatP= 2.70D-03

IDIUse=3 WtCom= 9.90D-01 WtEn= 9.61D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.304 Goal= None Shift= 0.000

Gap= 0.393 Goal= None Shift= 0.000

RMSDP=1.05D-04 MaxDP=3.49D-03 OVMax= 2.44D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.05D-04 CP: 1.00D+00

E= -1275.84228809497 Delta-E= -0.000972082421 Rises=F Damp=F

DIIS: error= 5.47D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84228809497 IErMin= 2 ErrMin= 5.47D-04

ErrMax= 5.47D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.29D-04 BMatP= 2.70D-03

IDIUse=3 WtCom= 9.95D-01 WtEn= 5.47D-03

Coeff-Com: 0.137D+00 0.863D+00

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

Coeff: 0.136D+00 0.864D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.57D-05 MaxDP=1.94D-03 DE=-9.72D-04 OVMax= 2.09D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.50D-05 CP: 1.00D+00 1.07D+00

E= -1275.84229681200 Delta-E= -0.000008717027 Rises=F Damp=F

DIIS: error= 8.17D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1275.84229681200 IErMin= 2 ErrMin= 5.47D-04

ErrMax= 8.17D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.91D-04 BMatP= 3.29D-04

IDIUse=3 WtCom= 2.59D-01 WtEn= 7.41D-01

Coeff-Com: -0.755D-02 0.582D+00 0.425D+00

Coeff-En: 0.000D+00 0.478D+00 0.522D+00

Coeff: -0.196D-02 0.505D+00 0.497D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.47D-05 MaxDP=1.33D-03 DE=-8.72D-06 OVMax= 5.71D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.10D-05 CP: 1.00D+00 1.14D+00 7.02D-01

E= -1275.84242942800 Delta-E= -0.000132616001 Rises=F Damp=F

DIIS: error= 4.26D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84242942800 IErMin= 4 ErrMin= 4.26D-04

ErrMax= 4.26D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.66D-05 BMatP= 3.29D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 4.26D-03

Coeff-Com: -0.776D-02 0.117D+00 0.279D+00 0.612D+00

Coeff-En: 0.000D+00 0.000D+00 0.376D-01 0.962D+00

Coeff: -0.772D-02 0.117D+00 0.278D+00 0.613D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.47D-05 MaxDP=7.99D-04 DE=-1.33D-04 OVMax= 9.86D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 6.75D-06 CP: 1.00D+00 1.16D+00 1.06D+00 1.09D+00

E= -1275.84246785732 Delta-E= -0.000038429317 Rises=F Damp=F

DIIS: error= 2.13D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84246785732 IErMin= 5 ErrMin= 2.13D-04

ErrMax= 2.13D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.34D-05 BMatP= 7.66D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.13D-03

Coeff-Com: -0.653D-03-0.617D-01 0.387D-01 0.353D+00 0.671D+00

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

Coeff: -0.652D-03-0.616D-01 0.386D-01 0.352D+00 0.671D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.19D-05 MaxDP=5.31D-04 DE=-3.84D-05 OVMax= 8.55D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.09D-06 CP: 1.00D+00 1.20D+00 1.27D+00 1.45D+00 1.33D+00

E= -1275.84248839474 Delta-E= -0.000020537421 Rises=F Damp=F

DIIS: error= 1.76D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84248839474 IErMin= 6 ErrMin= 1.76D-04

ErrMax= 1.76D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.06D-06 BMatP= 1.34D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.76D-03

Coeff-Com: 0.959D-02-0.135D+00-0.247D+00-0.270D+00 0.212D+00 0.143D+01

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

Coeff: 0.957D-02-0.135D+00-0.247D+00-0.270D+00 0.212D+00 0.143D+01

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.52D-05 MaxDP=1.26D-03 DE=-2.05D-05 OVMax= 1.88D-02

Cycle 7 Pass 1 IDiag 1:

RMSU= 3.37D-06 CP: 1.00D+00 1.28D+00 1.74D+00 2.15D+00 2.50D+00

CP: 2.10D+00

E= -1275.84251568043 Delta-E= -0.000027285689 Rises=F Damp=F

DIIS: error= 1.13D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84251568043 IErMin= 7 ErrMin= 1.13D-04

ErrMax= 1.13D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.41D-06 BMatP= 6.06D-06

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.13D-03

Coeff-Com: 0.846D-02-0.770D-01-0.240D+00-0.406D+00-0.229D+00 0.118D+01

Coeff-Com: 0.765D+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: 0.845D-02-0.769D-01-0.240D+00-0.406D+00-0.228D+00 0.118D+01

Coeff: 0.765D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.86D-05 MaxDP=8.95D-04 DE=-2.73D-05 OVMax= 1.38D-02

Cycle 8 Pass 1 IDiag 1:

RMSU= 3.00D-06 CP: 1.00D+00 1.33D+00 2.08D+00 2.68D+00 3.00D+00

CP: 3.00D+00 1.42D+00

E= -1275.84252471577 Delta-E= -0.000009035345 Rises=F Damp=F

DIIS: error= 3.36D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84252471577 IErMin= 8 ErrMin= 3.36D-05

ErrMax= 3.36D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.49D-07 BMatP= 4.41D-06

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

Coeff-Com: -0.264D-03 0.289D-01 0.158D-02-0.273D-01-0.122D+00-0.603D-01

Coeff-Com: 0.286D+00 0.894D+00

Coeff: -0.264D-03 0.289D-01 0.158D-02-0.273D-01-0.122D+00-0.603D-01

Coeff: 0.286D+00 0.894D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.00D-06 MaxDP=2.23D-04 DE=-9.04D-06 OVMax= 3.00D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.38D-06 CP: 1.00D+00 1.34D+00 2.14D+00 2.78D+00 3.00D+00

CP: 3.00D+00 1.79D+00 1.58D+00

E= -1275.84252560081 Delta-E= -0.000000885032 Rises=F Damp=F

DIIS: error= 1.67D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84252560081 IErMin= 9 ErrMin= 1.67D-05

ErrMax= 1.67D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.36D-07 BMatP= 6.49D-07

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

Coeff-Com: -0.207D-02 0.366D-01 0.567D-01 0.808D-01 0.387D-03-0.328D+00

Coeff-Com: -0.353D-01 0.542D+00 0.649D+00

Coeff: -0.207D-02 0.366D-01 0.567D-01 0.808D-01 0.387D-03-0.328D+00

Coeff: -0.353D-01 0.542D+00 0.649D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.49D-06 MaxDP=8.13D-05 DE=-8.85D-07 OVMax= 9.98D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 6.05D-07 CP: 1.00D+00 1.34D+00 2.16D+00 2.80D+00 3.00D+00

CP: 3.00D+00 1.94D+00 1.86D+00 1.22D+00

E= -1275.84252587130 Delta-E= -0.000000270490 Rises=F Damp=F

DIIS: error= 8.96D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84252587130 IErMin=10 ErrMin= 8.96D-06

ErrMax= 8.96D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.32D-08 BMatP= 3.36D-07

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

Coeff-Com: -0.559D-03 0.249D-02 0.160D-01 0.368D-01 0.511D-01-0.985D-01

Coeff-Com: -0.127D+00-0.560D-01 0.187D+00 0.988D+00

Coeff: -0.559D-03 0.249D-02 0.160D-01 0.368D-01 0.511D-01-0.985D-01

Coeff: -0.127D+00-0.560D-01 0.187D+00 0.988D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.24D-06 MaxDP=7.03D-05 DE=-2.70D-07 OVMax= 8.87D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 3.54D-07 CP: 1.00D+00 1.34D+00 2.18D+00 2.82D+00 3.00D+00

CP: 3.00D+00 2.07D+00 2.06D+00 1.52D+00 1.32D+00

E= -1275.84252598015 Delta-E= -0.000000108856 Rises=F Damp=F

DIIS: error= 6.16D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84252598015 IErMin=11 ErrMin= 6.16D-06

ErrMax= 6.16D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.75D-08 BMatP= 5.32D-08

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

Coeff-Com: 0.132D-03-0.662D-02-0.389D-02 0.598D-02 0.255D-01 0.213D-01

Coeff-Com: -0.722D-01-0.128D+00-0.690D-01 0.502D+00 0.725D+00

Coeff: 0.132D-03-0.662D-02-0.389D-02 0.598D-02 0.255D-01 0.213D-01

Coeff: -0.722D-01-0.128D+00-0.690D-01 0.502D+00 0.725D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=5.47D-07 MaxDP=2.89D-05 DE=-1.09D-07 OVMax= 3.67D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.74D-07 CP: 1.00D+00 1.34D+00 2.18D+00 2.84D+00 3.00D+00

CP: 3.00D+00 2.12D+00 2.13D+00 1.62D+00 1.65D+00

CP: 1.30D+00

E= -1275.84252600929 Delta-E= -0.000000029132 Rises=F Damp=F

DIIS: error= 3.12D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84252600929 IErMin=12 ErrMin= 3.12D-06

ErrMax= 3.12D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.25D-08 BMatP= 2.75D-08

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

Coeff-Com: 0.359D-03-0.578D-02-0.112D-01-0.129D-01-0.118D-01 0.644D-01

Coeff-Com: 0.448D-02-0.454D-01-0.148D+00-0.139D+00 0.499D+00 0.806D+00

Coeff: 0.359D-03-0.578D-02-0.112D-01-0.129D-01-0.118D-01 0.644D-01

Coeff: 0.448D-02-0.454D-01-0.148D+00-0.139D+00 0.499D+00 0.806D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=6.50D-07 MaxDP=3.43D-05 DE=-2.91D-08 OVMax= 4.89D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.10D-07 CP: 1.00D+00 1.34D+00 2.19D+00 2.85D+00 3.00D+00

CP: 3.00D+00 2.15D+00 2.22D+00 1.74D+00 1.84D+00

CP: 1.65D+00 1.09D+00

E= -1275.84252602530 Delta-E= -0.000000016017 Rises=F Damp=F

DIIS: error= 1.09D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84252602530 IErMin=13 ErrMin= 1.09D-06

ErrMax= 1.09D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.72D-09 BMatP= 1.25D-08

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

Coeff-Com: 0.135D-03-0.110D-02-0.410D-02-0.650D-02-0.124D-01 0.242D-01

Coeff-Com: 0.143D-01 0.911D-02-0.531D-01-0.182D+00 0.842D-01 0.378D+00

Coeff-Com: 0.750D+00

Coeff: 0.135D-03-0.110D-02-0.410D-02-0.650D-02-0.124D-01 0.242D-01

Coeff: 0.143D-01 0.911D-02-0.531D-01-0.182D+00 0.842D-01 0.378D+00

Coeff: 0.750D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.88D-07 MaxDP=1.46D-05 DE=-1.60D-08 OVMax= 2.17D-04

Cycle 14 Pass 1 IDiag 1:

RMSU= 4.45D-08 CP: 1.00D+00 1.35D+00 2.20D+00 2.86D+00 3.00D+00

CP: 3.00D+00 2.17D+00 2.26D+00 1.78D+00 1.89D+00

CP: 1.78D+00 1.28D+00 1.19D+00

E= -1275.84252602730 Delta-E= -0.000000002001 Rises=F Damp=F

DIIS: error= 5.03D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84252602730 IErMin=14 ErrMin= 5.03D-07

ErrMax= 5.03D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.78D-10 BMatP= 1.72D-09

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

Coeff-Com: -0.276D-05 0.747D-03 0.354D-03-0.459D-03-0.437D-02-0.117D-02

Coeff-Com: 0.705D-02 0.171D-01 0.628D-02-0.756D-01-0.682D-01 0.349D-01

Coeff-Com: 0.444D+00 0.639D+00

Coeff: -0.276D-05 0.747D-03 0.354D-03-0.459D-03-0.437D-02-0.117D-02

Coeff: 0.705D-02 0.171D-01 0.628D-02-0.756D-01-0.682D-01 0.349D-01

Coeff: 0.444D+00 0.639D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.53D-08 MaxDP=1.97D-06 DE=-2.00D-09 OVMax= 2.86D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 1.74D-08 CP: 1.00D+00 1.35D+00 2.20D+00 2.86D+00 3.00D+00

CP: 3.00D+00 2.17D+00 2.26D+00 1.78D+00 1.91D+00

CP: 1.82D+00 1.33D+00 1.31D+00 9.39D-01

E= -1275.84252602750 Delta-E= -0.000000000197 Rises=F Damp=F

DIIS: error= 1.89D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.84252602750 IErMin=15 ErrMin= 1.89D-07

ErrMax= 1.89D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.77D-11 BMatP= 4.78D-10

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

Coeff-Com: -0.158D-04 0.351D-03 0.533D-03 0.316D-03-0.979D-04-0.300D-02

Coeff-Com: 0.140D-02 0.442D-02 0.885D-02-0.707D-02-0.351D-01-0.306D-01

Coeff-Com: 0.635D-01 0.215D+00 0.782D+00

Coeff: -0.158D-04 0.351D-03 0.533D-03 0.316D-03-0.979D-04-0.300D-02

Coeff: 0.140D-02 0.442D-02 0.885D-02-0.707D-02-0.351D-01-0.306D-01

Coeff: 0.635D-01 0.215D+00 0.782D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.39D-08 MaxDP=9.28D-07 DE=-1.97D-10 OVMax= 7.09D-06

Cycle 16 Pass 1 IDiag 1:

RMSU= 7.70D-09 CP: 1.00D+00 1.35D+00 2.20D+00 2.86D+00 3.00D+00

CP: 3.00D+00 2.17D+00 2.26D+00 1.78D+00 1.91D+00

CP: 1.82D+00 1.34D+00 1.35D+00 1.01D+00 1.09D+00

E= -1275.84252602752 Delta-E= -0.000000000016 Rises=F Damp=F

DIIS: error= 1.23D-07 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1275.84252602752 IErMin=16 ErrMin= 1.23D-07

ErrMax= 1.23D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.40D-11 BMatP= 3.77D-11

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

Coeff-Com: -0.882D-05 0.331D-04 0.286D-03 0.438D-03 0.113D-02-0.150D-02

Coeff-Com: -0.111D-02-0.230D-02 0.292D-02 0.138D-01-0.444D-03-0.189D-01

Coeff-Com: -0.588D-01-0.497D-01 0.354D+00 0.760D+00

Coeff: -0.882D-05 0.331D-04 0.286D-03 0.438D-03 0.113D-02-0.150D-02

Coeff: -0.111D-02-0.230D-02 0.292D-02 0.138D-01-0.444D-03-0.189D-01

Coeff: -0.588D-01-0.497D-01 0.354D+00 0.760D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.92D-08 MaxDP=9.97D-07 DE=-1.59D-11 OVMax= 1.44D-05

Cycle 17 Pass 1 IDiag 1:

RMSU= 4.14D-09 CP: 1.00D+00 1.35D+00 2.20D+00 2.86D+00 3.00D+00

CP: 3.00D+00 2.17D+00 2.26D+00 1.78D+00 1.91D+00

CP: 1.83D+00 1.34D+00 1.35D+00 1.02D+00 1.25D+00

CP: 1.34D+00

E= -1275.84252602753 Delta-E= -0.000000000010 Rises=F Damp=F

DIIS: error= 7.03D-08 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=17 EnMin= -1275.84252602753 IErMin=17 ErrMin= 7.03D-08

ErrMax= 7.03D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.84D-12 BMatP= 1.40D-11

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

Coeff-Com: -0.251D-06-0.704D-04-0.139D-04 0.392D-04 0.503D-03 0.697D-04

Coeff-Com: -0.563D-03-0.202D-02-0.188D-03 0.809D-02 0.603D-02-0.368D-02

Coeff-Com: -0.396D-01-0.754D-01 0.238D-01 0.415D+00 0.668D+00

Coeff: -0.251D-06-0.704D-04-0.139D-04 0.392D-04 0.503D-03 0.697D-04

Coeff: -0.563D-03-0.202D-02-0.188D-03 0.809D-02 0.603D-02-0.368D-02

Coeff: -0.396D-01-0.754D-01 0.238D-01 0.415D+00 0.668D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.44D-09 MaxDP=2.17D-07 DE=-1.00D-11 OVMax= 2.82D-06

Error on total polarization charges = 0.06459

SCF Done: E(UB3LYP) = -1275.84252603 A.U. after 17 cycles

NFock= 17 Conv=0.44D-08 -V/T= 1.9659

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0176 S= 1.0058

<L.S>= 0.000000000000E+00

KE= 1.320856851276D+03 PE=-8.578004915283D+03 EE= 3.218296181114D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.72

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0176, after 2.0002

Leave Link 502 at Tue Sep 17 14:14:47 2019, MaxMem= 2415919104 cpu: 1549.6

(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= 15339 LenP2D= 41300.

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 = 248

Leave Link 701 at Tue Sep 17 14:14:51 2019, MaxMem= 2415919104 cpu: 70.4

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 14:14:51 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 14:15:01 2019, MaxMem= 2415919104 cpu: 177.6

(Enter /home/blab/g09/l716.exe)

Dipole = 6.94555524D-13-3.59712260D-14 4.44089210D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.001343526 -0.000333763 0.000000000

2 7 0.000549969 -0.000280295 -0.000000000

3 6 0.000075384 0.000235956 -0.000000000

4 6 -0.000733916 -0.000933598 0.000000000

5 6 0.000966232 -0.000268367 0.000000000

6 7 -0.003401804 -0.000491292 -0.000000000

7 6 0.003244571 0.002616764 0.000000000

8 7 0.000158730 -0.000367793 0.000000000

9 6 0.002406593 -0.004142278 -0.000000000

10 6 -0.000729258 0.001346023 -0.000000000

11 6 -0.000857442 -0.001614543 0.000000000

12 7 0.002619594 -0.002922164 0.000000000

13 6 0.000729258 -0.001346023 -0.000000000

14 6 0.000857442 0.001614543 0.000000000

15 6 -0.003244571 -0.002616764 -0.000000000

16 7 -0.000158730 0.000367793 -0.000000000

17 6 -0.002406593 0.004142278 -0.000000000

18 7 0.003401804 0.000491292 0.000000000

19 7 -0.000549969 0.000280295 0.000000000

20 6 -0.000075384 -0.000235956 0.000000000

21 6 0.000733916 0.000933598 0.000000000

22 6 -0.000966232 0.000268367 0.000000000

23 6 0.001343526 0.000333763 0.000000000

24 7 -0.002619594 0.002922164 0.000000000

25 30 0.000000000 -0.000000000 -0.000000000

26 6 0.000031208 -0.000376434 -0.000000000

27 1 0.000059942 0.000038183 -0.000000000

28 6 -0.000150462 -0.000127359 0.000000000

29 1 0.000405150 -0.000747952 -0.000000000

30 6 0.000150462 0.000127359 0.000000000

31 1 -0.000405150 0.000747952 0.000000000

32 6 -0.000031208 0.000376434 0.000000000

33 1 -0.000059942 -0.000038183 -0.000000000

34 1 -0.000248651 -0.000189149 0.000000000

35 1 0.000356703 -0.000236242 0.000594760

36 1 0.000356703 -0.000236242 -0.000594760

37 1 0.000080940 0.000194476 0.000571665

38 1 0.000080940 0.000194476 -0.000571665

39 1 -0.000008194 -0.000293007 0.000000000

40 1 -0.000080940 -0.000194476 0.000571665

41 1 -0.000080940 -0.000194476 -0.000571665

42 1 0.000008194 0.000293007 -0.000000000

43 1 -0.000356703 0.000236242 0.000594760

44 1 -0.000356703 0.000236242 -0.000594760

45 1 0.000248651 0.000189149 -0.000000000

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

Cartesian Forces: Max 0.004142278 RMS 0.001095919

Leave Link 716 at Tue Sep 17 14:15:01 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 0.003365217 RMS 0.000578679

Search for a local minimum.

Step number 14 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 12 13 14

DE= 1.32D-04 DEPred=-8.57D-04 R=-1.54D-01

Trust test=-1.54D-01 RLast= 9.09D-02 DXMaxT set to 1.58D-01

ITU= -1 1 1 1 -1 0 1 -1 1 1 1 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01337

Eigenvalues --- 0.01338 0.01347 0.01348 0.01604 0.01623

Eigenvalues --- 0.01631 0.01640 0.01775 0.01794 0.01809

Eigenvalues --- 0.01824 0.01891 0.01912 0.01940 0.01952

Eigenvalues --- 0.01997 0.02000 0.02045 0.02048 0.02070

Eigenvalues --- 0.02088 0.02103 0.02111 0.02115 0.02205

Eigenvalues --- 0.02311 0.02315 0.02350 0.02372 0.07029

Eigenvalues --- 0.07174 0.07174 0.07189 0.07189 0.07314

Eigenvalues --- 0.07320 0.07397 0.09373 0.13773 0.14499

Eigenvalues --- 0.14501 0.15266 0.15867 0.15945 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16020

Eigenvalues --- 0.16056 0.16357 0.17486 0.18526 0.20786

Eigenvalues --- 0.22053 0.22089 0.23839 0.23855 0.23886

Eigenvalues --- 0.24711 0.24897 0.24997 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.26091

Eigenvalues --- 0.27235 0.29752 0.31210 0.32550 0.33009

Eigenvalues --- 0.33189 0.33200 0.33282 0.33282 0.33485

Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33737 0.34327 0.34435 0.34437

Eigenvalues --- 0.34437 0.34547 0.34627 0.35554 0.35560

Eigenvalues --- 0.35682 0.35682 0.35685 0.35753 0.36426

Eigenvalues --- 0.38958 0.41617 0.41814 0.41981 0.44848

Eigenvalues --- 0.47570 0.48963 0.48980 0.49189 0.51357

Eigenvalues --- 0.51362 0.51502 0.52367 0.53840 0.54031

Eigenvalues --- 0.54036 0.56315 0.56321 0.56492

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 0.82220 0.17780

Cosine: 1.000 > 0.970

Length: 1.000

GDIIS step was calculated using 2 of the last 14 vectors.

Iteration 1 RMS(Cart)= 0.00496426 RMS(Int)= 0.00000721

Iteration 2 RMS(Cart)= 0.00000930 RMS(Int)= 0.00000241

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000241

ITry= 1 IFail=0 DXMaxC= 2.09D-02 DCOld= 1.00D+10 DXMaxT= 1.58D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 5.70D-10 for atom 6.

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

(Linear) (Quad) (Total)

R1 2.58004 0.00000 -0.00391 0.00683 0.00291 2.58296

R2 2.72995 0.00090 0.00184 0.00155 0.00339 2.73334

R3 2.59016 -0.00044 0.00316 -0.00713 -0.00397 2.58619

R4 2.56445 -0.00026 0.00190 -0.00477 -0.00288 2.56157

R5 3.79433 0.00135 0.00127 0.00209 0.00335 3.79768

R6 2.77011 0.00076 -0.00157 0.00644 0.00487 2.77498

R7 2.58408 -0.00155 -0.00054 -0.00407 -0.00461 2.57947

R8 2.59862 -0.00030 -0.00003 -0.00160 -0.00163 2.59699

R9 2.81034 0.00114 0.00150 0.00136 0.00286 2.81320

R10 2.04309 -0.00007 -0.00021 0.00004 -0.00018 2.04291

R11 2.49184 0.00207 -0.00091 0.00831 0.00740 2.49924

R12 2.58561 -0.00046 0.00236 -0.00615 -0.00378 2.58183

R13 2.80293 -0.00059 -0.00069 -0.00199 -0.00267 2.80025

R14 2.57699 -0.00015 -0.00335 0.00553 0.00218 2.57917

R15 3.77608 0.00132 0.00033 0.00490 0.00523 3.78131

R16 2.84454 -0.00028 0.00256 -0.00706 -0.00450 2.84005

R17 2.48193 0.00337 0.00255 0.00454 0.00709 2.48902

R18 2.54639 0.00133 -0.00045 0.00413 0.00369 2.55008

R19 2.80651 -0.00001 -0.00033 0.00084 0.00050 2.80702

R20 2.04121 0.00085 0.00116 0.00102 0.00218 2.04339

R21 2.48193 0.00337 0.00255 0.00454 0.00709 2.48902

R22 2.54639 0.00133 -0.00045 0.00413 0.00369 2.55008

R23 2.84454 -0.00028 0.00256 -0.00706 -0.00450 2.84005

R24 2.80651 -0.00001 -0.00033 0.00084 0.00050 2.80702

R25 2.80293 -0.00059 -0.00069 -0.00199 -0.00267 2.80025

R26 2.04121 0.00085 0.00116 0.00102 0.00218 2.04339

R27 2.58561 -0.00046 0.00236 -0.00615 -0.00378 2.58183

R28 2.49184 0.00207 -0.00091 0.00831 0.00740 2.49924

R29 2.57699 -0.00015 -0.00335 0.00553 0.00218 2.57917

R30 3.77608 0.00132 0.00033 0.00490 0.00523 3.78131

R31 2.58408 -0.00155 -0.00054 -0.00407 -0.00461 2.57947

R32 2.56445 -0.00026 0.00190 -0.00477 -0.00288 2.56157

R33 2.58004 0.00000 -0.00391 0.00683 0.00291 2.58296

R34 3.79433 0.00135 0.00127 0.00209 0.00335 3.79768

R35 2.77011 0.00076 -0.00157 0.00644 0.00487 2.77498

R36 2.59862 -0.00030 -0.00003 -0.00160 -0.00163 2.59699

R37 2.81034 0.00114 0.00150 0.00136 0.00286 2.81320

R38 2.72995 0.00090 0.00184 0.00155 0.00339 2.73334

R39 2.04309 -0.00007 -0.00021 0.00004 -0.00018 2.04291

R40 2.59016 -0.00044 0.00316 -0.00713 -0.00397 2.58619

R41 2.06143 0.00031 0.00041 0.00047 0.00088 2.06231

R42 2.06752 0.00073 0.00083 0.00112 0.00196 2.06948

R43 2.06752 0.00073 0.00083 0.00112 0.00196 2.06948

R44 2.06712 0.00058 0.00089 0.00073 0.00162 2.06874

R45 2.06712 0.00058 0.00089 0.00073 0.00162 2.06874

R46 2.06093 0.00022 0.00023 0.00036 0.00058 2.06151

R47 2.06712 0.00058 0.00089 0.00073 0.00162 2.06874

R48 2.06712 0.00058 0.00089 0.00073 0.00162 2.06874

R49 2.06093 0.00022 0.00023 0.00036 0.00058 2.06151

R50 2.06752 0.00073 0.00083 0.00112 0.00196 2.06948

R51 2.06752 0.00073 0.00083 0.00112 0.00196 2.06948

R52 2.06143 0.00031 0.00041 0.00047 0.00088 2.06231

A1 1.89379 0.00007 0.00010 -0.00190 -0.00180 1.89199

A2 2.20719 -0.00076 -0.00075 -0.00140 -0.00215 2.20504

A3 2.18221 0.00069 0.00065 0.00329 0.00395 2.18615

A4 1.90742 -0.00066 -0.00122 0.00052 -0.00069 1.90673

A5 2.19280 0.00025 0.00117 -0.00241 -0.00125 2.19155

A6 2.18297 0.00042 0.00005 0.00189 0.00194 2.18491

A7 1.89269 0.00111 0.00242 0.00069 0.00311 1.89581

A8 2.22565 -0.00062 -0.00190 0.00064 -0.00126 2.22438

A9 2.16485 -0.00049 -0.00052 -0.00133 -0.00185 2.16300

A10 1.85501 -0.00099 -0.00256 -0.00098 -0.00354 1.85147

A11 2.17294 0.00039 0.00220 -0.00115 0.00105 2.17399

A12 2.25524 0.00060 0.00037 0.00213 0.00249 2.25773

A13 1.87587 0.00048 0.00126 0.00166 0.00291 1.87878

A14 2.18287 -0.00024 -0.00026 -0.00147 -0.00173 2.18114

A15 2.22445 -0.00023 -0.00100 -0.00018 -0.00118 2.22326

A16 2.16360 0.00124 0.00277 0.00015 0.00291 2.16651

A17 2.23431 -0.00084 -0.00080 -0.00210 -0.00290 2.23141

A18 2.16853 -0.00013 -0.00062 -0.00035 -0.00097 2.16755

A19 1.88035 0.00097 0.00142 0.00245 0.00388 1.88422

A20 1.91573 -0.00030 -0.00032 -0.00140 -0.00172 1.91401

A21 2.18892 0.00003 -0.00078 0.00177 0.00100 2.18992

A22 2.17853 0.00027 0.00110 -0.00038 0.00072 2.17926

A23 1.88420 0.00009 -0.00055 0.00045 -0.00010 1.88410

A24 2.25408 -0.00158 -0.00054 -0.00683 -0.00736 2.24672

A25 2.14491 0.00150 0.00109 0.00637 0.00746 2.15237

A26 1.85540 0.00018 0.00144 0.00019 0.00163 1.85703

A27 2.15251 0.00018 -0.00081 0.00324 0.00243 2.15495

A28 2.27527 -0.00035 -0.00063 -0.00344 -0.00406 2.27121

A29 1.88911 -0.00093 -0.00198 -0.00170 -0.00368 1.88542

A30 2.16242 0.00045 0.00074 0.00203 0.00276 2.16519

A31 2.23166 0.00049 0.00124 -0.00032 0.00092 2.23258

A32 2.16310 0.00159 -0.00032 0.00867 0.00835 2.17146

A33 1.85540 0.00018 0.00144 0.00019 0.00163 1.85703

A34 2.27527 -0.00035 -0.00063 -0.00344 -0.00406 2.27121

A35 2.15251 0.00018 -0.00081 0.00324 0.00243 2.15495

A36 1.88911 -0.00093 -0.00198 -0.00170 -0.00368 1.88542

A37 2.23166 0.00049 0.00124 -0.00032 0.00092 2.23258

A38 2.16242 0.00045 0.00074 0.00203 0.00276 2.16519

A39 1.88035 0.00097 0.00142 0.00245 0.00388 1.88422

A40 2.16853 -0.00013 -0.00062 -0.00035 -0.00097 2.16755

A41 2.23431 -0.00084 -0.00080 -0.00210 -0.00290 2.23141

A42 1.91573 -0.00030 -0.00032 -0.00140 -0.00172 1.91401

A43 2.18892 0.00003 -0.00078 0.00177 0.00100 2.18992

A44 2.17853 0.00027 0.00110 -0.00038 0.00072 2.17926

A45 2.14491 0.00150 0.00109 0.00637 0.00746 2.15237

A46 2.25408 -0.00158 -0.00054 -0.00683 -0.00736 2.24672

A47 1.88420 0.00009 -0.00055 0.00045 -0.00010 1.88410

A48 2.16360 0.00124 0.00277 0.00015 0.00291 2.16651

A49 1.90742 -0.00066 -0.00122 0.00052 -0.00069 1.90673

A50 2.18297 0.00042 0.00005 0.00189 0.00194 2.18491

A51 2.19280 0.00025 0.00117 -0.00241 -0.00125 2.19155

A52 2.22565 -0.00062 -0.00190 0.00064 -0.00126 2.22438

A53 2.16485 -0.00049 -0.00052 -0.00133 -0.00185 2.16300

A54 1.89269 0.00111 0.00242 0.00069 0.00311 1.89581

A55 1.85501 -0.00099 -0.00256 -0.00098 -0.00354 1.85147

A56 2.17294 0.00039 0.00220 -0.00115 0.00105 2.17399

A57 2.25524 0.00060 0.00037 0.00213 0.00249 2.25773

A58 1.87587 0.00048 0.00126 0.00166 0.00291 1.87878

A59 2.22445 -0.00023 -0.00100 -0.00018 -0.00118 2.22326

A60 2.18287 -0.00024 -0.00026 -0.00147 -0.00173 2.18114

A61 1.89379 0.00007 0.00010 -0.00190 -0.00180 1.89199

A62 2.20719 -0.00076 -0.00075 -0.00140 -0.00215 2.20504

A63 2.18221 0.00069 0.00065 0.00329 0.00395 2.18615

A64 2.16310 0.00159 -0.00032 0.00867 0.00835 2.17146

A65 1.57092 -0.00023 0.00066 -0.00234 -0.00168 1.56925

A66 1.57067 0.00023 -0.00066 0.00234 0.00168 1.57235

A67 1.57067 0.00023 -0.00066 0.00234 0.00168 1.57235

A68 1.57092 -0.00023 0.00066 -0.00234 -0.00168 1.56925

A69 1.94394 -0.00008 -0.00045 -0.00033 -0.00078 1.94316

A70 1.94012 0.00011 0.00058 0.00005 0.00064 1.94076

A71 1.94012 0.00011 0.00058 0.00005 0.00064 1.94076

A72 1.88993 -0.00006 -0.00016 -0.00009 -0.00025 1.88969

A73 1.88993 -0.00006 -0.00016 -0.00009 -0.00025 1.88969

A74 1.85660 -0.00002 -0.00043 0.00043 0.00000 1.85660

A75 1.93369 -0.00001 0.00056 0.00018 0.00074 1.93443

A76 1.93369 -0.00001 0.00056 0.00018 0.00074 1.93443

A77 1.94799 -0.00031 -0.00112 -0.00179 -0.00291 1.94508

A78 1.85506 0.00019 -0.00030 0.00210 0.00180 1.85686

A79 1.89522 0.00009 0.00016 -0.00025 -0.00009 1.89513

A80 1.89522 0.00009 0.00016 -0.00025 -0.00009 1.89513

A81 1.93369 -0.00001 0.00056 0.00018 0.00074 1.93443

A82 1.93369 -0.00001 0.00056 0.00018 0.00074 1.93443

A83 1.94799 -0.00031 -0.00112 -0.00179 -0.00291 1.94508

A84 1.85506 0.00019 -0.00030 0.00210 0.00180 1.85686

A85 1.89522 0.00009 0.00016 -0.00025 -0.00009 1.89513

A86 1.89522 0.00009 0.00016 -0.00025 -0.00009 1.89513

A87 1.94012 0.00011 0.00058 0.00005 0.00064 1.94076

A88 1.94012 0.00011 0.00058 0.00005 0.00064 1.94076

A89 1.94394 -0.00008 -0.00045 -0.00033 -0.00078 1.94316

A90 1.85660 -0.00002 -0.00043 0.00043 0.00000 1.85660

A91 1.88993 -0.00006 -0.00016 -0.00009 -0.00025 1.88969

A92 1.88993 -0.00006 -0.00016 -0.00009 -0.00025 1.88969

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

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D21 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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D66 -2.11434 0.00011 0.00017 0.00142 0.00158 -2.11275

D67 2.11434 -0.00011 -0.00017 -0.00142 -0.00158 2.11275

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D80 2.11434 -0.00011 -0.00017 -0.00142 -0.00158 2.11275

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D125 1.03231 0.00006 0.00011 0.00030 0.00041 1.03273

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D127 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D128 -2.10928 0.00006 0.00011 0.00030 0.00041 -2.10886

D129 2.10928 -0.00006 -0.00011 -0.00030 -0.00041 2.10886

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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 0.003365 0.000450 NO

RMS Force 0.000579 0.000300 NO

Maximum Displacement 0.020929 0.001800 NO

RMS Displacement 0.004962 0.001200 NO

Predicted change in Energy=-1.617136D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:15:01 2019, MaxMem= 2415919104 cpu: 1.3

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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1 6 0 -2.072895 -2.192134 0.000000

2 7 0 -0.745467 -1.866265 0.000000

3 6 0 -0.006396 -3.002585 0.000000

4 6 0 -0.917279 -4.154389 0.000000

5 6 0 -2.189159 -3.633876 0.000000

6 7 0 1.354562 -3.107484 0.000000

7 6 0 2.178573 -2.073014 0.000000

8 7 0 1.857068 -0.745134 0.000000

9 6 0 2.998137 0.003693 0.000000

10 6 0 4.169816 -0.937498 0.000000

11 6 0 3.656140 -2.185349 0.000000

12 7 0 -3.123294 -1.314866 0.000000

13 6 0 -4.169816 0.937498 0.000000

14 6 0 -3.656140 2.185349 0.000000

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16 7 0 -1.857068 0.745134 0.000000

17 6 0 -2.998137 -0.003693 0.000000

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22 6 0 2.189159 3.633876 0.000000

23 6 0 2.072895 2.192134 0.000000

24 7 0 3.123294 1.314866 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.479503 -5.577247 0.000000

27 1 0 -3.121976 -4.180274 0.000000

28 6 0 5.584463 -0.484494 0.000000

29 1 0 4.192024 -3.124535 0.000000

30 6 0 -5.584463 0.484494 0.000000

31 1 0 -4.192024 3.124535 0.000000

32 6 0 0.479503 5.577247 0.000000

33 1 0 3.121976 4.180274 0.000000

34 1 0 -1.334339 -6.255665 0.000000

35 1 0 0.137057 -5.801840 0.876755

36 1 0 0.137057 -5.801840 -0.876755

37 1 0 5.794334 0.136862 0.876527

38 1 0 5.794334 0.136862 -0.876527

39 1 0 6.273961 -1.329873 0.000000

40 1 0 -5.794334 -0.136862 0.876527

41 1 0 -5.794334 -0.136862 -0.876527

42 1 0 -6.273961 1.329873 0.000000

43 1 0 -0.137057 5.801840 0.876755

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45 1 0 1.334339 6.255665 0.000000

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Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.366841 0.000000

3 C 2.219740 1.355525 0.000000

4 C 2.277256 2.294566 1.468455 0.000000

5 C 1.446422 2.282257 2.272220 1.374268 0.000000

6 N 3.547580 2.439415 1.364995 2.501454 3.582603

7 C 4.253136 2.931340 2.374488 3.730472 4.638251

8 N 4.187889 2.833747 2.927215 4.395455 4.971598

9 C 5.526031 4.184652 4.250285 5.711403 6.335609

10 C 6.367539 5.002261 4.658899 6.018881 6.907027

11 C 5.729038 4.413157 3.752605 4.979285 6.022105

12 N 1.368553 2.440922 3.544495 3.595747 2.500083

13 C 3.767184 4.425749 5.732217 6.042045 4.982014

14 C 4.655000 4.988746 6.343129 6.906058 6.001284

15 C 4.266458 4.191863 5.520875 6.353851 5.706901

16 N 2.945187 2.838144 4.179759 4.988841 4.391585

17 C 2.375994 2.922960 4.236020 4.643086 3.719231

18 N 5.348079 5.010905 6.257035 7.275027 6.792826

19 N 4.941029 4.019286 4.926561 6.246039 6.234066

20 C 5.595405 4.926561 6.005184 7.216333 6.990214

21 C 7.015661 6.246039 7.216333 8.508902 8.384929

22 C 7.218553 6.234066 6.990214 8.384929 8.484686

23 C 6.034018 4.941029 5.595405 7.015661 7.218553

24 N 6.268925 5.008682 5.332480 6.799925 7.260317

25 Zn 3.017009 2.009643 3.002592 4.254451 4.242343

26 C 3.741375 3.720500 2.617768 1.488681 2.588361

27 H 2.247949 3.316992 3.330734 2.204849 1.081063

28 C 7.845455 6.478989 6.131761 7.465975 8.387360

29 H 6.333923 5.095298 4.200191 5.212061 6.401479

30 C 4.415365 5.379772 6.578339 6.580414 5.337514

31 H 5.723432 6.065216 7.420315 7.981647 7.048942

32 C 8.177898 7.543634 8.593580 9.831365 9.589919

33 H 8.221574 7.177587 7.834551 9.261868 9.448233

34 H 4.130103 4.428725 3.513682 2.142265 2.757625

35 H 4.322333 4.127505 2.936853 2.143459 3.298492

36 H 4.322333 4.127505 2.936853 2.143459 3.298492

37 H 8.251413 6.895638 6.653789 8.014293 8.872595

38 H 8.251413 6.895638 6.653789 8.014293 8.872595

39 H 8.391275 7.039893 6.499297 7.726049 8.771137

40 H 4.340686 5.408345 6.517737 6.379224 5.098500

41 H 4.340686 5.408345 6.517737 6.379224 5.098500

42 H 5.482107 6.385887 7.619223 7.666236 6.428407

43 H 8.271626 7.742009 8.848937 10.025166 9.696008

44 H 8.271626 7.742009 8.848937 10.025166 9.696008

45 H 9.109037 8.383993 9.354826 10.650776 10.498479

6 7 8 9 10

6 N 0.000000

7 C 1.322543 0.000000

8 N 2.415203 1.366247 0.000000

9 C 3.518630 2.232577 1.364837 0.000000

10 C 3.554504 2.292258 2.320734 1.502888 0.000000

11 C 2.479434 1.481831 2.304534 2.285798 1.349443

12 N 4.823346 5.355798 5.012843 6.261829 7.302866

13 C 6.846943 7.026039 6.257362 7.228522 8.547811

14 C 7.288430 7.223401 6.243652 7.002786 8.426016

15 C 6.270614 6.014505 4.922231 5.574981 7.026039

16 N 5.015699 4.922231 4.001963 4.911492 6.257362

17 C 5.345980 5.574981 4.911492 5.996278 7.228522

18 N 6.779762 6.270614 5.015699 5.345980 6.846943

19 N 5.010905 4.191863 2.838144 2.922960 4.425749

20 C 6.257035 5.520875 4.179759 4.236020 5.732217

21 C 7.275027 6.353851 4.988841 4.643086 6.042045

22 C 6.792826 5.706901 4.391585 3.719231 4.982014

23 C 5.348079 4.266458 2.945187 2.375994 3.767184

24 N 4.762939 3.517134 2.418042 1.317133 2.483616

25 Zn 3.389881 3.007253 2.000982 2.998139 4.273905

26 C 3.076284 4.398296 5.367390 6.575779 6.568366

27 H 4.603289 5.704065 6.049055 7.413593 7.980340

28 C 4.977162 3.758123 3.736496 2.631997 1.485409

29 H 2.837514 2.271493 3.333701 3.348309 2.187150

30 C 7.813601 8.173467 7.542438 8.596056 9.857384

31 H 8.342821 8.221862 7.180937 7.838244 9.296261

32 C 8.728704 7.836666 6.470718 6.116209 7.487343

33 H 7.499011 6.324052 5.085238 4.178417 5.223941

34 H 4.140197 5.462153 6.367969 7.612484 7.653668

35 H 3.083922 4.340579 5.412708 6.531362 6.379159

36 H 3.083922 4.340579 5.412708 6.531362 6.379159

37 H 5.568273 4.327307 4.128956 2.933386 2.135792

38 H 5.568273 4.327307 4.128956 2.933386 2.135792

39 H 5.230716 4.162267 4.455431 3.536867 2.140417

40 H 7.790995 8.251317 7.725429 8.837171 10.034620

41 H 7.790995 8.251317 7.725429 8.837171 10.034620

42 H 8.825219 9.111804 8.391621 9.366459 10.687069

43 H 9.075774 8.254949 6.899863 6.649560 8.045902

44 H 9.075774 8.254949 6.899863 6.649560 8.045902

45 H 9.363171 8.371358 7.020288 6.469574 7.731851

11 12 13 14 15

11 C 0.000000

12 N 6.835090 0.000000

13 C 8.426016 2.483616 0.000000

14 C 8.518945 3.540541 1.349443 0.000000

15 C 7.223401 3.517134 2.292258 1.481831 0.000000

16 N 6.243652 2.418042 2.320734 2.304534 1.366247

17 C 7.002786 1.317133 1.502888 2.285798 2.232577

18 N 7.288430 4.762939 3.554504 2.479434 1.322543

19 N 4.988746 5.008682 5.002261 4.413157 2.931340

20 C 6.343129 5.332480 4.658899 3.752605 2.374488

21 C 6.906058 6.799925 6.018881 4.979285 3.730472

22 C 6.001284 7.260317 6.907027 6.022105 4.638251

23 C 4.655000 6.268925 6.367539 5.729038 4.253136

24 N 3.540541 6.777562 7.302866 6.835090 5.355798

25 Zn 4.259473 3.388781 4.273905 4.259473 3.007253

26 C 5.348693 5.015727 7.487343 8.387426 7.836666

27 H 7.065591 2.865409 5.223941 6.387996 6.324052

28 C 2.571252 8.747259 9.857384 9.618565 8.173467

29 H 1.081315 7.535833 9.296261 9.475682 8.221862

30 C 9.618565 3.048778 1.485409 2.571252 3.758123

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32 C 8.387426 7.776976 6.568366 5.348693 4.398296

33 H 6.387996 8.318651 7.980340 7.065591 5.704065

34 H 6.439903 5.254699 7.731851 8.754512 8.371358

35 H 5.121684 5.615294 8.045902 8.885507 8.254949

36 H 5.121684 5.615294 8.045902 8.885507 8.254949

37 H 3.276101 9.077439 10.034620 9.709586 8.251317

38 H 3.276101 9.077439 10.034620 9.709586 8.251317

39 H 2.754057 9.397267 10.687069 10.533930 9.111804

40 H 9.709586 3.048024 2.135792 3.276101 4.327307

41 H 9.709586 3.048024 2.135792 3.276101 4.327307

42 H 10.533930 4.113557 2.140417 2.754057 4.162267

43 H 8.885507 7.767484 6.379159 5.121684 4.340579

44 H 8.885507 7.767484 6.379159 5.121684 4.340579

45 H 8.754512 8.785410 7.653668 6.439903 5.462153

16 17 18 19 20

16 N 0.000000

17 C 1.364837 0.000000

18 N 2.415203 3.518630 0.000000

19 N 2.833747 4.184652 2.439415 0.000000

20 C 2.927215 4.250285 1.364995 1.355525 0.000000

21 C 4.395455 5.711403 2.501454 2.294566 1.468455

22 C 4.971598 6.335609 3.582603 2.282257 2.272220

23 C 4.187889 5.526031 3.547580 1.366841 2.219740

24 N 5.012843 6.261829 4.823346 2.440922 3.544495

25 Zn 2.000982 2.998139 3.389881 2.009643 3.002592

26 C 6.470718 6.116209 8.728704 7.543634 8.593580

27 H 5.085238 4.178417 7.499011 7.177587 7.834551

28 C 7.542438 8.596056 7.813601 5.379772 6.578339

29 H 7.180937 7.838244 8.342821 6.065216 7.420315

30 C 3.736496 2.631997 4.977162 6.478989 6.131761

31 H 3.333701 3.348309 2.837514 5.095298 4.200191

32 C 5.367390 6.575779 3.076284 3.720500 2.617768

33 H 6.049055 7.413593 4.603289 3.316992 3.330734

34 H 7.020288 6.469574 9.363171 8.383993 9.354826

35 H 6.899863 6.649560 9.075774 7.742009 8.848937

36 H 6.899863 6.649560 9.075774 7.742009 8.848937

37 H 7.725429 8.837171 7.790995 5.408345 6.517737

38 H 7.725429 8.837171 7.790995 5.408345 6.517737

39 H 8.391621 9.366459 8.825219 6.385887 7.619223

40 H 4.128956 2.933386 5.568273 6.895638 6.653789

41 H 4.128956 2.933386 5.568273 6.895638 6.653789

42 H 4.455431 3.536867 5.230716 7.039893 6.499297

43 H 5.412708 6.531362 3.083922 4.127505 2.936853

44 H 5.412708 6.531362 3.083922 4.127505 2.936853

45 H 6.367969 7.612484 4.140197 4.428725 3.513682

21 22 23 24 25

21 C 0.000000

22 C 1.374268 0.000000

23 C 2.277256 1.446422 0.000000

24 N 3.595747 2.500083 1.368553 0.000000

25 Zn 4.254451 4.242343 3.017009 3.388781 0.000000

26 C 9.831365 9.589919 8.177898 7.776976 5.597821

27 H 9.261868 9.448233 8.221574 8.318651 5.217416

28 C 6.580414 5.337514 4.415365 3.048778 5.605440

29 H 7.981647 7.048942 5.723432 4.566231 5.228363

30 C 7.465975 8.387360 7.845455 8.747259 5.605440

31 H 5.212061 6.401479 6.333923 7.535833 5.228363

32 C 1.488681 2.588361 3.741375 5.015727 5.597821

33 H 2.204849 1.081063 2.247949 2.865409 5.217416

34 H 10.650776 10.498479 9.109037 8.785410 6.396390

35 H 10.025166 9.696008 8.271626 7.767484 5.869313

36 H 10.025166 9.696008 8.271626 7.767484 5.869313

37 H 6.379224 5.098500 4.340686 3.048024 5.861855

38 H 6.379224 5.098500 4.340686 3.048024 5.861855

39 H 7.666236 6.428407 5.482107 4.113557 6.413357

40 H 8.014293 8.872595 8.251413 9.077439 5.861855

41 H 8.014293 8.872595 8.251413 9.077439 5.861855

42 H 7.726049 8.771137 8.391275 9.397267 6.413357

43 H 2.143459 3.298492 4.322333 5.615294 5.869313

44 H 2.143459 3.298492 4.322333 5.615294 5.869313

45 H 2.142265 2.757625 4.130103 5.254699 6.396390

26 27 28 29 30

26 C 0.000000

27 H 2.989012 0.000000

28 C 7.918827 9.458376 0.000000

29 H 5.276264 7.389803 2.984745 0.000000

30 C 7.924980 5.274837 11.210880 10.421362 0.000000

31 H 9.460645 7.382767 10.421362 10.456727 2.984745

32 C 11.195643 10.400955 7.924980 9.460645 7.918827

33 H 10.400955 10.434832 5.274837 7.382767 9.458376

34 H 1.091328 2.739141 9.009786 6.351745 7.968268

35 H 1.095121 3.744259 7.662708 4.937552 8.545320

36 H 1.095121 3.744259 7.662708 4.937552 8.545320

37 H 8.531141 9.945178 1.094728 3.737968 11.417801

38 H 8.531141 9.945178 1.094728 3.737968 11.417801

39 H 7.978062 9.818779 1.090905 2.748686 11.996422

40 H 7.655946 4.925341 11.417801 10.460490 1.094728

41 H 7.655946 4.925341 11.417801 10.460490 1.094728

42 H 9.015766 6.347971 11.996422 11.374471 1.090905

43 H 11.417950 10.455671 8.545320 9.959408 7.662708

44 H 11.417950 10.455671 8.545320 9.959408 7.662708

45 H 11.971125 11.347580 7.968268 9.805841 9.009786

31 32 33 34 35

31 H 0.000000

32 C 5.276264 0.000000

33 H 7.389803 2.989012 0.000000

34 H 9.805841 11.971125 11.347580 0.000000

35 H 9.959408 11.417950 10.455671 1.771910 0.000000

36 H 9.959408 11.417950 10.455671 1.771910 1.753511

37 H 10.460490 7.655946 4.925341 9.615128 8.202010

38 H 10.460490 7.655946 4.925341 9.615128 8.387310

39 H 11.374471 9.015766 6.347971 9.063645 7.643872

40 H 3.737968 8.531141 9.945178 7.622310 8.202035

41 H 3.737968 8.531141 9.945178 7.622310 8.387335

42 H 2.748686 7.978062 9.818779 9.052086 9.629703

43 H 4.937552 1.095121 3.744259 12.148482 11.606918

44 H 4.937552 1.095121 3.744259 12.148482 11.738626

45 H 6.351745 1.091328 2.739141 12.792781 12.148482

36 37 38 39 40

36 H 0.000000

37 H 8.387310 0.000000

38 H 8.202010 1.753055 0.000000

39 H 7.643872 1.774726 1.774726 0.000000

40 H 8.387335 11.591901 11.723710 12.158755 0.000000

41 H 8.202035 11.723710 11.591901 12.158755 1.753055

42 H 9.629703 12.158755 12.158755 12.826715 1.774726

43 H 11.738626 8.202035 8.387335 9.629703 8.202010

44 H 11.606918 8.387335 8.202035 9.629703 8.387310

45 H 12.148482 7.622310 7.622310 9.052086 9.615128

41 42 43 44 45

41 H 0.000000

42 H 1.774726 0.000000

43 H 8.387310 7.643872 0.000000

44 H 8.202010 7.643872 1.753511 0.000000

45 H 9.615128 9.063645 1.771910 1.771910 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=0 Diff= 2.99D-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 2.806386 -1.107493 0.000000

2 7 0 2.009641 0.003116 0.000000

3 6 0 2.789017 1.112179 0.000000

4 6 0 4.197180 0.695723 0.000000

5 6 0 4.187731 -0.678513 0.000000

6 7 0 2.379572 2.414318 0.000000

7 6 0 1.112654 2.793845 0.000000

8 7 0 0.000000 2.000982 0.000000

9 6 0 -1.119886 2.781131 0.000000

10 6 0 -0.682703 4.219026 0.000000

11 6 0 0.666686 4.206975 0.000000

12 7 0 2.383365 -2.409026 0.000000

13 6 0 0.682703 -4.219026 0.000000

14 6 0 -0.666686 -4.206975 0.000000

15 6 0 -1.112654 -2.793845 0.000000

16 7 0 -0.000000 -2.000982 0.000000

17 6 0 1.119886 -2.781131 0.000000

18 7 0 -2.379572 -2.414318 0.000000

19 7 0 -2.009641 -0.003116 0.000000

20 6 0 -2.789017 -1.112179 0.000000

21 6 0 -4.197180 -0.695723 0.000000

22 6 0 -4.187731 0.678513 0.000000

23 6 0 -2.806386 1.107493 0.000000

24 7 0 -2.383365 2.409026 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 5.354683 1.631863 0.000000

27 1 0 5.042198 -1.340770 0.000000

28 6 0 -1.629918 5.363238 0.000000

29 1 0 1.338770 5.054056 0.000000

30 6 0 1.629918 -5.363238 0.000000

31 1 0 -1.338770 -5.054056 0.000000

32 6 0 -5.354683 -1.631863 0.000000

33 1 0 -5.042198 1.340770 0.000000

34 1 0 6.302636 1.091141 0.000000

35 1 0 5.333526 2.287715 0.876755

36 1 0 5.333526 2.287715 -0.876755

37 1 0 -2.284738 5.326632 0.876527

38 1 0 -2.284738 5.326632 -0.876527

39 1 0 -1.102099 6.317953 0.000000

40 1 0 2.284738 -5.326632 0.876527

41 1 0 2.284738 -5.326632 -0.876527

42 1 0 1.102099 -6.317953 0.000000

43 1 0 -5.333526 -2.287715 0.876755

44 1 0 -5.333526 -2.287715 -0.876755

45 1 0 -6.302636 -1.091141 0.000000

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

Rotational constants (GHZ): 0.1829082 0.1818867 0.0914024

Leave Link 202 at Tue Sep 17 14:15:01 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 101 beta electrons

nuclear repulsion energy 2761.5012768674 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= -0.1142094551 Hartrees.

Nuclear repulsion after empirical dispersion term = 2761.3870674124 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 = 3498

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.69D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 130

GePol: Fraction of low-weight points (<1% of avg) = 3.72%

GePol: Cavity surface area = 382.122 Ang\*\*2

GePol: Cavity volume = 379.341 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0107046513 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2761.3763627611 Hartrees.

Leave Link 301 at Tue Sep 17 14:15:01 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= 15325 LenP2D= 41262.

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 14:15:02 2019, MaxMem= 2415919104 cpu: 12.6

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:15:02 2019, MaxMem= 2415919104 cpu: 1.2

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= -0.000000 -0.000000 -0.000000

Rot= 1.000000 -0.000000 -0.000000 -0.000183 Ang= -0.02 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 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0176 S= 1.0059

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= -1276.14930716134

Leave Link 401 at Tue Sep 17 14:15:05 2019, MaxMem= 2415919104 cpu: 39.8

(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= 36708012.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.33D-15 for 3472.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.50D-15 for 1529 1041.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.44D-15 for 3472.

Iteration 1 A^-1\*A deviation from orthogonality is 1.05D-11 for 1758 1748.

E= -1275.84253326699

DIIS: error= 3.80D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.84253326699 IErMin= 1 ErrMin= 3.80D-04

ErrMax= 3.80D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.13D-04 BMatP= 4.13D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.80D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.303 Goal= None Shift= 0.000

Gap= 0.393 Goal= None Shift= 0.000

RMSDP=3.28D-05 MaxDP=6.26D-04 OVMax= 5.35D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.28D-05 CP: 1.00D+00

E= -1275.84266102200 Delta-E= -0.000127755011 Rises=F Damp=F

DIIS: error= 1.04D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84266102200 IErMin= 2 ErrMin= 1.04D-04

ErrMax= 1.04D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.51D-05 BMatP= 4.13D-04

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.04D-03

Coeff-Com: 0.646D-01 0.935D+00

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

Coeff: 0.645D-01 0.935D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=8.39D-06 MaxDP=3.54D-04 DE=-1.28D-04 OVMax= 4.03D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 8.16D-06 CP: 1.00D+00 1.06D+00

E= -1275.84266207356 Delta-E= -0.000001051551 Rises=F Damp=F

DIIS: error= 1.28D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1275.84266207356 IErMin= 2 ErrMin= 1.04D-04

ErrMax= 1.28D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.06D-05 BMatP= 2.51D-05

IDIUse=3 WtCom= 4.69D-01 WtEn= 5.31D-01

Coeff-Com: -0.131D-01 0.531D+00 0.482D+00

Coeff-En: 0.000D+00 0.451D+00 0.549D+00

Coeff: -0.616D-02 0.489D+00 0.518D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.41D-06 MaxDP=2.72D-04 DE=-1.05D-06 OVMax= 9.71D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 3.59D-06 CP: 1.00D+00 1.08D+00 6.97D-01

E= -1275.84266821143 Delta-E= -0.000006137872 Rises=F Damp=F

DIIS: error= 8.53D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84266821143 IErMin= 4 ErrMin= 8.53D-05

ErrMax= 8.53D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.02D-06 BMatP= 2.51D-05

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

Coeff-Com: -0.971D-02 0.152D+00 0.274D+00 0.583D+00

Coeff: -0.971D-02 0.152D+00 0.274D+00 0.583D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.60D-06 MaxDP=1.34D-04 DE=-6.14D-06 OVMax= 1.75D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.89D-06 CP: 1.00D+00 1.09D+00 9.10D-01 1.05D+00

E= -1275.84266927248 Delta-E= -0.000001061047 Rises=F Damp=F

DIIS: error= 4.20D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84266927248 IErMin= 5 ErrMin= 4.20D-05

ErrMax= 4.20D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.69D-07 BMatP= 3.02D-06

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

Coeff-Com: -0.410D-02 0.377D-01 0.113D+00 0.389D+00 0.465D+00

Coeff: -0.410D-02 0.377D-01 0.113D+00 0.389D+00 0.465D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.34D-06 MaxDP=6.00D-05 DE=-1.06D-06 OVMax= 8.99D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 6.28D-07 CP: 1.00D+00 1.10D+00 9.90D-01 1.31D+00 1.10D+00

E= -1275.84266967340 Delta-E= -0.000000400924 Rises=F Damp=F

DIIS: error= 3.30D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84266967340 IErMin= 6 ErrMin= 3.30D-05

ErrMax= 3.30D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.49D-07 BMatP= 6.69D-07

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

Coeff-Com: 0.266D-02-0.553D-01-0.883D-01-0.450D-01 0.361D-01 0.115D+01

Coeff: 0.266D-02-0.553D-01-0.883D-01-0.450D-01 0.361D-01 0.115D+01

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.72D-06 MaxDP=1.49D-04 DE=-4.01D-07 OVMax= 2.15D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 4.80D-07 CP: 1.00D+00 1.11D+00 1.18D+00 1.76D+00 1.81D+00

CP: 1.84D+00

E= -1275.84267018291 Delta-E= -0.000000509513 Rises=F Damp=F

DIIS: error= 2.14D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84267018291 IErMin= 7 ErrMin= 2.14D-05

ErrMax= 2.14D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.33D-07 BMatP= 1.49D-07

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

Coeff-Com: 0.389D-02-0.519D-01-0.122D+00-0.204D+00-0.368D+00 0.757D+00

Coeff-Com: 0.985D+00

Coeff: 0.389D-02-0.519D-01-0.122D+00-0.204D+00-0.368D+00 0.757D+00

Coeff: 0.985D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.92D-06 MaxDP=1.52D-04 DE=-5.10D-07 OVMax= 2.27D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 3.01D-07 CP: 1.00D+00 1.12D+00 1.37D+00 2.25D+00 2.51D+00

CP: 3.00D+00 1.74D+00

E= -1275.84267056613 Delta-E= -0.000000383215 Rises=F Damp=F

DIIS: error= 1.30D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84267056613 IErMin= 8 ErrMin= 1.30D-05

ErrMax= 1.30D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.31D-08 BMatP= 1.33D-07

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

Coeff-Com: -0.653D-04 0.167D-01-0.138D-02-0.284D-01-0.270D+00-0.251D+00

Coeff-Com: 0.425D+00 0.111D+01

Coeff: -0.653D-04 0.167D-01-0.138D-02-0.284D-01-0.270D+00-0.251D+00

Coeff: 0.425D+00 0.111D+01

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.43D-06 MaxDP=1.29D-04 DE=-3.83D-07 OVMax= 1.90D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 6.91D-07 CP: 1.00D+00 1.13D+00 1.52D+00 2.66D+00 3.00D+00

CP: 3.00D+00 2.71D+00 2.04D+00

E= -1275.84267073829 Delta-E= -0.000000172167 Rises=F Damp=F

DIIS: error= 6.39D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84267073829 IErMin= 9 ErrMin= 6.39D-06

ErrMax= 6.39D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.85D-08 BMatP= 4.31D-08

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

Coeff-Com: -0.129D-02 0.266D-01 0.380D-01 0.554D-01-0.476D-01-0.389D+00

Coeff-Com: -0.138D+00 0.663D+00 0.793D+00

Coeff: -0.129D-02 0.266D-01 0.380D-01 0.554D-01-0.476D-01-0.389D+00

Coeff: -0.138D+00 0.663D+00 0.793D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.28D-06 MaxDP=6.73D-05 DE=-1.72D-07 OVMax= 9.82D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 4.89D-07 CP: 1.00D+00 1.14D+00 1.60D+00 2.87D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.88D+00 1.75D+00

E= -1275.84267077816 Delta-E= -0.000000039867 Rises=F Damp=F

DIIS: error= 2.62D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84267077816 IErMin=10 ErrMin= 2.62D-06

ErrMax= 2.62D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.78D-09 BMatP= 1.85D-08

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

Coeff-Com: -0.749D-03 0.990D-02 0.230D-01 0.472D-01 0.713D-01-0.114D+00

Coeff-Com: -0.240D+00-0.360D-02 0.443D+00 0.764D+00

Coeff: -0.749D-03 0.990D-02 0.230D-01 0.472D-01 0.713D-01-0.114D+00

Coeff: -0.240D+00-0.360D-02 0.443D+00 0.764D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.35D-07 MaxDP=1.76D-05 DE=-3.99D-08 OVMax= 2.44D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.22D-07 CP: 1.00D+00 1.14D+00 1.62D+00 2.91D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.94D+00 1.24D+00

E= -1275.84267078358 Delta-E= -0.000000005419 Rises=F Damp=F

DIIS: error= 1.08D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84267078358 IErMin=11 ErrMin= 1.08D-06

ErrMax= 1.08D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.38D-09 BMatP= 4.78D-09

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

Coeff-Com: -0.331D-04-0.269D-02 0.124D-02 0.936D-02 0.523D-01 0.508D-01

Coeff-Com: -0.954D-01-0.183D+00 0.810D-02 0.431D+00 0.729D+00

Coeff: -0.331D-04-0.269D-02 0.124D-02 0.936D-02 0.523D-01 0.508D-01

Coeff: -0.954D-01-0.183D+00 0.810D-02 0.431D+00 0.729D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.34D-07 MaxDP=7.78D-06 DE=-5.42D-09 OVMax= 9.03D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 5.02D-08 CP: 1.00D+00 1.14D+00 1.63D+00 2.93D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.03D+00 1.35D+00

CP: 1.31D+00

E= -1275.84267078487 Delta-E= -0.000000001288 Rises=F Damp=F

DIIS: error= 5.62D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84267078487 IErMin=12 ErrMin= 5.62D-07

ErrMax= 5.62D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.96D-10 BMatP= 1.38D-09

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

Coeff-Com: 0.136D-03-0.342D-02-0.440D-02-0.663D-02 0.780D-02 0.473D-01

Coeff-Com: 0.733D-02-0.858D-01-0.947D-01 0.491D-01 0.348D+00 0.735D+00

Coeff: 0.136D-03-0.342D-02-0.440D-02-0.663D-02 0.780D-02 0.473D-01

Coeff: 0.733D-02-0.858D-01-0.947D-01 0.491D-01 0.348D+00 0.735D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=6.96D-08 MaxDP=3.49D-06 DE=-1.29D-09 OVMax= 4.71D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.92D-08 CP: 1.00D+00 1.14D+00 1.63D+00 2.94D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.06D+00 1.41D+00

CP: 1.51D+00 1.21D+00

E= -1275.84267078518 Delta-E= -0.000000000307 Rises=F Damp=F

DIIS: error= 3.88D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84267078518 IErMin=13 ErrMin= 3.88D-07

ErrMax= 3.88D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.26D-11 BMatP= 2.96D-10

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

Coeff-Com: 0.835D-04-0.914D-03-0.243D-02-0.606D-02-0.116D-01 0.110D-01

Coeff-Com: 0.313D-01 0.103D-01-0.538D-01-0.103D+00-0.413D-01 0.376D+00

Coeff-Com: 0.790D+00

Coeff: 0.835D-04-0.914D-03-0.243D-02-0.606D-02-0.116D-01 0.110D-01

Coeff: 0.313D-01 0.103D-01-0.538D-01-0.103D+00-0.413D-01 0.376D+00

Coeff: 0.790D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.48D-08 MaxDP=2.12D-06 DE=-3.07D-10 OVMax= 1.10D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 1.36D-08 CP: 1.00D+00 1.14D+00 1.64D+00 2.95D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.07D+00 1.42D+00

CP: 1.59D+00 1.44D+00 1.34D+00

E= -1275.84267078529 Delta-E= -0.000000000116 Rises=F Damp=F

DIIS: error= 2.23D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84267078529 IErMin=14 ErrMin= 2.23D-07

ErrMax= 2.23D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.86D-11 BMatP= 9.26D-11

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

Coeff-Com: -0.756D-05 0.776D-03 0.406D-03-0.790D-03-0.893D-02-0.113D-01

Coeff-Com: 0.126D-01 0.375D-01 0.545D-02-0.696D-01-0.144D+00-0.735D-01

Coeff-Com: 0.390D+00 0.861D+00

Coeff: -0.756D-05 0.776D-03 0.406D-03-0.790D-03-0.893D-02-0.113D-01

Coeff: 0.126D-01 0.375D-01 0.545D-02-0.696D-01-0.144D+00-0.735D-01

Coeff: 0.390D+00 0.861D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.57D-08 MaxDP=1.34D-06 DE=-1.16D-10 OVMax= 6.40D-06

Cycle 15 Pass 1 IDiag 1:

RMSU= 5.76D-09 CP: 1.00D+00 1.14D+00 1.64D+00 2.95D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.08D+00 1.42D+00

CP: 1.64D+00 1.58D+00 1.79D+00 1.35D+00

E= -1275.84267078532 Delta-E= -0.000000000029 Rises=F Damp=F

DIIS: error= 9.40D-08 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.84267078532 IErMin=15 ErrMin= 9.40D-08

ErrMax= 9.40D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.95D-12 BMatP= 2.86D-11

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

Coeff-Com: -0.249D-04 0.651D-03 0.834D-03 0.999D-03-0.201D-02-0.925D-02

Coeff-Com: -0.118D-02 0.184D-01 0.160D-01-0.133D-01-0.673D-01-0.130D+00

Coeff-Com: 0.689D-02 0.490D+00 0.689D+00

Coeff: -0.249D-04 0.651D-03 0.834D-03 0.999D-03-0.201D-02-0.925D-02

Coeff: -0.118D-02 0.184D-01 0.160D-01-0.133D-01-0.673D-01-0.130D+00

Coeff: 0.689D-02 0.490D+00 0.689D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=8.17D-09 MaxDP=6.21D-07 DE=-2.91D-11 OVMax= 3.71D-06

Error on total polarization charges = 0.06464

SCF Done: E(UB3LYP) = -1275.84267079 A.U. after 15 cycles

NFock= 15 Conv=0.82D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0179 S= 1.0059

<L.S>= 0.000000000000E+00

KE= 1.320796307345D+03 PE=-8.574698192110D+03 EE= 3.216682851219D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.72

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0179, after 2.0002

Leave Link 502 at Tue Sep 17 14:16:23 2019, MaxMem= 2415919104 cpu: 1382.5

(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= 15325 LenP2D= 41262.

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 = 246

Leave Link 701 at Tue Sep 17 14:16:28 2019, MaxMem= 2415919104 cpu: 72.3

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 14:16:28 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 14:16:37 2019, MaxMem= 2415919104 cpu: 178.4

(Enter /home/blab/g09/l716.exe)

Dipole =-8.34887715D-14-6.79456491D-14-1.33226763D-15

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000213037 -0.000373260 -0.000000000

2 7 -0.000554027 -0.000509695 0.000000000

3 6 -0.000057910 -0.000515587 -0.000000000

4 6 0.000317089 0.000329328 -0.000000000

5 6 -0.000308939 0.000429945 0.000000000

6 7 0.000532872 0.000799774 0.000000000

7 6 -0.000358979 -0.000860034 0.000000000

8 7 0.000602147 0.000173011 -0.000000000

9 6 -0.000145959 0.000505422 -0.000000000

10 6 0.000282532 0.000042635 -0.000000000

11 6 -0.000113291 0.000054898 0.000000000

12 7 0.000058763 0.000768534 -0.000000000

13 6 -0.000282532 -0.000042635 0.000000000

14 6 0.000113291 -0.000054898 0.000000000

15 6 0.000358979 0.000860034 0.000000000

16 7 -0.000602147 -0.000173011 -0.000000000

17 6 0.000145959 -0.000505422 -0.000000000

18 7 -0.000532872 -0.000799774 0.000000000

19 7 0.000554027 0.000509695 -0.000000000

20 6 0.000057910 0.000515587 0.000000000

21 6 -0.000317089 -0.000329328 0.000000000

22 6 0.000308939 -0.000429945 -0.000000000

23 6 -0.000213037 0.000373260 0.000000000

24 7 -0.000058763 -0.000768534 0.000000000

25 30 0.000000000 -0.000000000 0.000000000

26 6 0.000150559 0.000045597 0.000000000

27 1 -0.000090852 0.000017308 0.000000000

28 6 0.000041240 0.000123712 0.000000000

29 1 -0.000036616 0.000056081 0.000000000

30 6 -0.000041240 -0.000123712 0.000000000

31 1 0.000036616 -0.000056081 0.000000000

32 6 -0.000150559 -0.000045597 -0.000000000

33 1 0.000090852 -0.000017308 0.000000000

34 1 -0.000019771 0.000003695 0.000000000

35 1 -0.000031734 0.000009464 0.000063349

36 1 -0.000031734 0.000009464 -0.000063349

37 1 -0.000037916 -0.000034047 0.000055466

38 1 -0.000037916 -0.000034047 -0.000055466

39 1 0.000009702 -0.000021015 0.000000000

40 1 0.000037916 0.000034047 0.000055466

41 1 0.000037916 0.000034047 -0.000055466

42 1 -0.000009702 0.000021015 -0.000000000

43 1 0.000031734 -0.000009464 0.000063349

44 1 0.000031734 -0.000009464 -0.000063349

45 1 0.000019771 -0.000003695 0.000000000

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

Cartesian Forces: Max 0.000860034 RMS 0.000265000

Leave Link 716 at Tue Sep 17 14:16:38 2019, MaxMem= 2415919104 cpu: 0.4

(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 0.000624893 RMS 0.000123403

Search for a local minimum.

Step number 15 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 12 13 14 15

DE= -1.45D-04 DEPred=-1.62D-04 R= 8.95D-01

TightC=F SS= 1.41D+00 RLast= 3.73D-02 DXNew= 2.6636D-01 1.1177D-01

Trust test= 8.95D-01 RLast= 3.73D-02 DXMaxT set to 1.58D-01

ITU= 1 -1 1 1 1 -1 0 1 -1 1 1 1 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01336

Eigenvalues --- 0.01338 0.01346 0.01347 0.01604 0.01623

Eigenvalues --- 0.01631 0.01639 0.01774 0.01793 0.01809

Eigenvalues --- 0.01823 0.01890 0.01909 0.01939 0.01950

Eigenvalues --- 0.01997 0.02000 0.02045 0.02047 0.02070

Eigenvalues --- 0.02087 0.02103 0.02110 0.02115 0.02205

Eigenvalues --- 0.02312 0.02316 0.02351 0.02372 0.02933

Eigenvalues --- 0.07146 0.07192 0.07192 0.07195 0.07195

Eigenvalues --- 0.07313 0.07374 0.07387 0.13742 0.14315

Eigenvalues --- 0.14497 0.14500 0.15737 0.15924 0.15980

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16022 0.16238 0.16999 0.18493 0.20540

Eigenvalues --- 0.22060 0.22091 0.23829 0.23842 0.23853

Eigenvalues --- 0.24087 0.24821 0.24974 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25075

Eigenvalues --- 0.26547 0.29281 0.31084 0.32631 0.33185

Eigenvalues --- 0.33189 0.33197 0.33282 0.33282 0.33441

Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33746 0.34100 0.34432 0.34437

Eigenvalues --- 0.34437 0.34463 0.35418 0.35555 0.35564

Eigenvalues --- 0.35636 0.35682 0.35682 0.35828 0.36387

Eigenvalues --- 0.38581 0.41346 0.41641 0.41815 0.44012

Eigenvalues --- 0.47672 0.48966 0.48981 0.49826 0.51276

Eigenvalues --- 0.51358 0.51361 0.53622 0.54020 0.54028

Eigenvalues --- 0.54355 0.56319 0.56329 0.57177

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 1.30466 0.03666 -0.07747 -0.05967 -0.38350

DIIS coeff's: 0.18637 -0.10434 0.17763 -0.05891 -0.02143

Cosine: 0.915 > 0.000

Length: 1.619

GDIIS step was calculated using 10 of the last 15 vectors.

Iteration 1 RMS(Cart)= 0.00070463 RMS(Int)= 0.00000536

Iteration 2 RMS(Cart)= 0.00000151 RMS(Int)= 0.00000533

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000533

ITry= 1 IFail=0 DXMaxC= 3.25D-03 DCOld= 1.00D+10 DXMaxT= 1.58D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 2.09D-10 for atom 33.

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

(Linear) (Quad) (Total)

R1 2.58296 -0.00022 -0.00315 -0.00017 -0.00330 2.57966

R2 2.73334 -0.00041 -0.00018 -0.00010 -0.00028 2.73306

R3 2.58619 0.00013 0.00229 -0.00021 0.00208 2.58827

R4 2.56157 -0.00000 0.00256 -0.00030 0.00227 2.56384

R5 3.79768 0.00023 0.00183 0.00027 0.00212 3.79980

R6 2.77498 -0.00032 -0.00249 0.00037 -0.00213 2.77285

R7 2.57947 0.00029 0.00043 -0.00003 0.00039 2.57986

R8 2.59699 0.00040 0.00100 0.00000 0.00099 2.59798

R9 2.81320 -0.00005 0.00022 -0.00002 0.00020 2.81340

R10 2.04291 0.00007 0.00025 -0.00004 0.00021 2.04312

R11 2.49924 -0.00059 -0.00260 -0.00026 -0.00287 2.49637

R12 2.58183 0.00009 0.00244 -0.00004 0.00239 2.58422

R13 2.80025 0.00002 -0.00042 0.00017 -0.00025 2.80001

R14 2.57917 -0.00019 -0.00272 -0.00024 -0.00297 2.57620

R15 3.78131 0.00031 0.00225 0.00020 0.00245 3.78376

R16 2.84005 0.00004 0.00176 0.00014 0.00191 2.84196

R17 2.48902 -0.00062 -0.00092 0.00002 -0.00092 2.48810

R18 2.55008 0.00011 0.00021 -0.00023 -0.00003 2.55005

R19 2.80702 -0.00001 -0.00006 -0.00015 -0.00021 2.80680

R20 2.04339 -0.00007 -0.00009 -0.00006 -0.00015 2.04324

R21 2.48902 -0.00062 -0.00092 0.00002 -0.00092 2.48810

R22 2.55008 0.00011 0.00021 -0.00023 -0.00003 2.55005

R23 2.84005 0.00004 0.00176 0.00014 0.00191 2.84196

R24 2.80702 -0.00001 -0.00006 -0.00015 -0.00021 2.80680

R25 2.80025 0.00002 -0.00042 0.00017 -0.00025 2.80001

R26 2.04339 -0.00007 -0.00009 -0.00006 -0.00015 2.04324

R27 2.58183 0.00009 0.00244 -0.00004 0.00239 2.58422

R28 2.49924 -0.00059 -0.00260 -0.00026 -0.00287 2.49637

R29 2.57917 -0.00019 -0.00272 -0.00024 -0.00297 2.57620

R30 3.78131 0.00031 0.00225 0.00020 0.00245 3.78376

R31 2.57947 0.00029 0.00043 -0.00003 0.00039 2.57986

R32 2.56157 -0.00000 0.00256 -0.00030 0.00227 2.56384

R33 2.58296 -0.00022 -0.00315 -0.00017 -0.00330 2.57966

R34 3.79768 0.00023 0.00183 0.00027 0.00212 3.79980

R35 2.77498 -0.00032 -0.00249 0.00037 -0.00213 2.77285

R36 2.59699 0.00040 0.00100 0.00000 0.00099 2.59798

R37 2.81320 -0.00005 0.00022 -0.00002 0.00020 2.81340

R38 2.73334 -0.00041 -0.00018 -0.00010 -0.00028 2.73306

R39 2.04291 0.00007 0.00025 -0.00004 0.00021 2.04312

R40 2.58619 0.00013 0.00229 -0.00021 0.00208 2.58827

R41 2.06231 0.00001 0.00010 -0.00003 0.00006 2.06237

R42 2.06948 0.00003 0.00022 -0.00017 0.00005 2.06953

R43 2.06948 0.00003 0.00022 -0.00017 0.00005 2.06953

R44 2.06874 0.00002 0.00030 -0.00021 0.00009 2.06882

R45 2.06874 0.00002 0.00030 -0.00021 0.00009 2.06882

R46 2.06151 0.00002 0.00015 -0.00006 0.00008 2.06159

R47 2.06874 0.00002 0.00030 -0.00021 0.00009 2.06882

R48 2.06874 0.00002 0.00030 -0.00021 0.00009 2.06882

R49 2.06151 0.00002 0.00015 -0.00006 0.00008 2.06159

R50 2.06948 0.00003 0.00022 -0.00017 0.00005 2.06953

R51 2.06948 0.00003 0.00022 -0.00017 0.00005 2.06953

R52 2.06231 0.00001 0.00010 -0.00003 0.00006 2.06237

A1 1.89199 -0.00002 -0.00025 0.00048 0.00025 1.89224

A2 2.20504 -0.00001 0.00057 -0.00043 0.00014 2.20518

A3 2.18615 0.00003 -0.00032 -0.00005 -0.00039 2.18576

A4 1.90673 0.00027 0.00104 -0.00021 0.00083 1.90756

A5 2.19155 -0.00008 0.00035 0.00034 0.00069 2.19224

A6 2.18491 -0.00019 -0.00140 -0.00013 -0.00152 2.18339

A7 1.89581 -0.00026 -0.00113 0.00002 -0.00110 1.89470

A8 2.22438 -0.00005 -0.00080 -0.00025 -0.00105 2.22333

A9 2.16300 0.00030 0.00193 0.00023 0.00215 2.16515

A10 1.85147 0.00012 0.00048 0.00008 0.00055 1.85202

A11 2.17399 -0.00015 0.00019 -0.00035 -0.00015 2.17383

A12 2.25773 0.00004 -0.00067 0.00027 -0.00040 2.25733

A13 1.87878 -0.00011 -0.00014 -0.00038 -0.00052 1.87826

A14 2.18114 -0.00001 -0.00000 0.00008 0.00008 2.18122

A15 2.22326 0.00012 0.00015 0.00029 0.00044 2.22370

A16 2.16651 0.00028 0.00274 0.00056 0.00328 2.16979

A17 2.23141 -0.00002 -0.00040 -0.00007 -0.00048 2.23093

A18 2.16755 0.00016 0.00133 0.00033 0.00166 2.16921

A19 1.88422 -0.00014 -0.00093 -0.00026 -0.00118 1.88304

A20 1.91401 0.00011 0.00082 0.00026 0.00107 1.91508

A21 2.18992 -0.00012 -0.00129 -0.00033 -0.00162 2.18830

A22 2.17926 0.00001 0.00047 0.00007 0.00054 2.17980

A23 1.88410 0.00005 -0.00004 -0.00011 -0.00014 1.88395

A24 2.24672 0.00000 0.00083 -0.00011 0.00071 2.24743

A25 2.15237 -0.00005 -0.00078 0.00022 -0.00057 2.15180

A26 1.85703 -0.00011 -0.00032 -0.00001 -0.00034 1.85669

A27 2.15495 -0.00002 -0.00032 -0.00022 -0.00055 2.15440

A28 2.27121 0.00013 0.00064 0.00024 0.00088 2.27209

A29 1.88542 0.00009 0.00047 0.00012 0.00059 1.88601

A30 2.16519 -0.00005 -0.00022 -0.00004 -0.00026 2.16493

A31 2.23258 -0.00004 -0.00025 -0.00008 -0.00033 2.23225

A32 2.17146 0.00017 -0.00106 0.00036 -0.00070 2.17075

A33 1.85703 -0.00011 -0.00032 -0.00001 -0.00034 1.85669

A34 2.27121 0.00013 0.00064 0.00024 0.00088 2.27209

A35 2.15495 -0.00002 -0.00032 -0.00022 -0.00055 2.15440

A36 1.88542 0.00009 0.00047 0.00012 0.00059 1.88601

A37 2.23258 -0.00004 -0.00025 -0.00008 -0.00033 2.23225

A38 2.16519 -0.00005 -0.00022 -0.00004 -0.00026 2.16493

A39 1.88422 -0.00014 -0.00093 -0.00026 -0.00118 1.88304

A40 2.16755 0.00016 0.00133 0.00033 0.00166 2.16921

A41 2.23141 -0.00002 -0.00040 -0.00007 -0.00048 2.23093

A42 1.91401 0.00011 0.00082 0.00026 0.00107 1.91508

A43 2.18992 -0.00012 -0.00129 -0.00033 -0.00162 2.18830

A44 2.17926 0.00001 0.00047 0.00007 0.00054 2.17980

A45 2.15237 -0.00005 -0.00078 0.00022 -0.00057 2.15180

A46 2.24672 0.00000 0.00083 -0.00011 0.00071 2.24743

A47 1.88410 0.00005 -0.00004 -0.00011 -0.00014 1.88395

A48 2.16651 0.00028 0.00274 0.00056 0.00328 2.16979

A49 1.90673 0.00027 0.00104 -0.00021 0.00083 1.90756

A50 2.18491 -0.00019 -0.00140 -0.00013 -0.00152 2.18339

A51 2.19155 -0.00008 0.00035 0.00034 0.00069 2.19224

A52 2.22438 -0.00005 -0.00080 -0.00025 -0.00105 2.22333

A53 2.16300 0.00030 0.00193 0.00023 0.00215 2.16515

A54 1.89581 -0.00026 -0.00113 0.00002 -0.00110 1.89470

A55 1.85147 0.00012 0.00048 0.00008 0.00055 1.85202

A56 2.17399 -0.00015 0.00019 -0.00035 -0.00015 2.17383

A57 2.25773 0.00004 -0.00067 0.00027 -0.00040 2.25733

A58 1.87878 -0.00011 -0.00014 -0.00038 -0.00052 1.87826

A59 2.22326 0.00012 0.00015 0.00029 0.00044 2.22370

A60 2.18114 -0.00001 -0.00000 0.00008 0.00008 2.18122

A61 1.89199 -0.00002 -0.00025 0.00048 0.00025 1.89224

A62 2.20504 -0.00001 0.00057 -0.00043 0.00014 2.20518

A63 2.18615 0.00003 -0.00032 -0.00005 -0.00039 2.18576

A64 2.17146 0.00017 -0.00106 0.00036 -0.00070 2.17075

A65 1.56925 0.00009 0.00115 0.00023 0.00138 1.57063

A66 1.57235 -0.00009 -0.00115 -0.00023 -0.00138 1.57096

A67 1.57235 -0.00009 -0.00115 -0.00023 -0.00138 1.57096

A68 1.56925 0.00009 0.00115 0.00023 0.00138 1.57063

A69 1.94316 -0.00003 -0.00054 0.00020 -0.00034 1.94281

A70 1.94076 -0.00003 0.00011 -0.00013 -0.00002 1.94074

A71 1.94076 -0.00003 0.00011 -0.00013 -0.00002 1.94074

A72 1.88969 0.00001 -0.00015 -0.00008 -0.00024 1.88945

A73 1.88969 0.00001 -0.00015 -0.00008 -0.00024 1.88945

A74 1.85660 0.00007 0.00066 0.00022 0.00089 1.85749

A75 1.93443 -0.00006 -0.00012 -0.00030 -0.00042 1.93401

A76 1.93443 -0.00006 -0.00012 -0.00030 -0.00042 1.93401

A77 1.94508 0.00001 0.00000 0.00014 0.00015 1.94523

A78 1.85686 0.00009 0.00026 0.00036 0.00062 1.85748

A79 1.89513 0.00002 -0.00001 0.00006 0.00006 1.89518

A80 1.89513 0.00002 -0.00001 0.00006 0.00006 1.89518

A81 1.93443 -0.00006 -0.00012 -0.00030 -0.00042 1.93401

A82 1.93443 -0.00006 -0.00012 -0.00030 -0.00042 1.93401

A83 1.94508 0.00001 0.00000 0.00014 0.00015 1.94523

A84 1.85686 0.00009 0.00026 0.00036 0.00062 1.85748

A85 1.89513 0.00002 -0.00001 0.00006 0.00006 1.89518

A86 1.89513 0.00002 -0.00001 0.00006 0.00006 1.89518

A87 1.94076 -0.00003 0.00011 -0.00013 -0.00002 1.94074

A88 1.94076 -0.00003 0.00011 -0.00013 -0.00002 1.94074

A89 1.94316 -0.00003 -0.00054 0.00020 -0.00034 1.94281

A90 1.85660 0.00007 0.00066 0.00022 0.00089 1.85749

A91 1.88969 0.00001 -0.00015 -0.00008 -0.00024 1.88945

A92 1.88969 0.00001 -0.00015 -0.00008 -0.00024 1.88945

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 1.03273 0.00003 0.00050 0.00005 0.00055 1.03328

D31 -1.03273 -0.00003 -0.00050 -0.00005 -0.00055 -1.03328

D32 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.10886 0.00003 0.00050 0.00005 0.00055 -2.10832

D34 2.10886 -0.00003 -0.00050 -0.00005 -0.00055 2.10832

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 1.02884 0.00002 0.00009 0.00003 0.00012 1.02896

D64 -1.02884 -0.00002 -0.00009 -0.00003 -0.00012 -1.02896

D65 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D66 -2.11275 0.00002 0.00009 0.00003 0.00012 -2.11264

D67 2.11275 -0.00002 -0.00009 -0.00003 -0.00012 2.11264

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 -2.11275 0.00002 0.00009 0.00003 0.00012 -2.11264

D80 2.11275 -0.00002 -0.00009 -0.00003 -0.00012 2.11264

D81 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D82 1.02884 0.00002 0.00009 0.00003 0.00012 1.02896

D83 -1.02884 -0.00002 -0.00009 -0.00003 -0.00012 -1.02896

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 1.03273 0.00003 0.00050 0.00005 0.00055 1.03328

D126 -1.03273 -0.00003 -0.00050 -0.00005 -0.00055 -1.03328

D127 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D128 -2.10886 0.00003 0.00050 0.00005 0.00055 -2.10832

D129 2.10886 -0.00003 -0.00050 -0.00005 -0.00055 2.10832

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 0.000625 0.000450 NO

RMS Force 0.000123 0.000300 YES

Maximum Displacement 0.003246 0.001800 NO

RMS Displacement 0.000704 0.001200 YES

Predicted change in Energy=-2.454069D-06

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:16:38 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 -2.072919 -2.192236 0.000000

2 7 0 -0.747185 -1.866789 0.000000

3 6 0 -0.006525 -3.003506 0.000000

4 6 0 -0.917030 -4.154172 0.000000

5 6 0 -2.189536 -3.633801 0.000000

6 7 0 1.354835 -3.105869 0.000000

7 6 0 2.179349 -2.073747 0.000000

8 7 0 1.858784 -0.744341 0.000000

9 6 0 2.998432 0.003787 0.000000

10 6 0 4.170901 -0.938035 0.000000

11 6 0 3.656814 -2.185699 0.000000

12 7 0 -3.124284 -1.314406 0.000000

13 6 0 -4.170901 0.938035 0.000000

14 6 0 -3.656814 2.185699 0.000000

15 6 0 -2.179349 2.073747 0.000000

16 7 0 -1.858784 0.744341 0.000000

17 6 0 -2.998432 -0.003787 0.000000

18 7 0 -1.354835 3.105869 0.000000

19 7 0 0.747185 1.866789 0.000000

20 6 0 0.006525 3.003506 0.000000

21 6 0 0.917030 4.154172 0.000000

22 6 0 2.189536 3.633801 0.000000

23 6 0 2.072919 2.192236 0.000000

24 7 0 3.124284 1.314406 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.479406 -5.577185 0.000000

27 1 0 -3.122542 -4.180095 0.000000

28 6 0 5.585192 -0.484291 0.000000

29 1 0 4.192653 -3.124818 0.000000

30 6 0 -5.585192 0.484291 0.000000

31 1 0 -4.192653 3.124818 0.000000

32 6 0 0.479406 5.577185 0.000000

33 1 0 3.122542 4.180095 0.000000

34 1 0 -1.334587 -6.255222 0.000000

35 1 0 0.136681 -5.801985 0.877071

36 1 0 0.136681 -5.801985 -0.877071

37 1 0 5.794324 0.137056 0.876769

38 1 0 5.794324 0.137056 -0.876769

39 1 0 6.275308 -1.329222 0.000000

40 1 0 -5.794324 -0.137056 0.876769

41 1 0 -5.794324 -0.137056 -0.876769

42 1 0 -6.275308 1.329222 0.000000

43 1 0 -0.136681 5.801985 0.877071

44 1 0 -0.136681 5.801985 -0.877071

45 1 0 1.334587 6.255222 0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.365097 0.000000

3 C 2.219942 1.356725 0.000000

4 C 2.277119 2.293680 1.467328 0.000000

5 C 1.446274 2.280944 2.272181 1.374793 0.000000

6 N 3.547425 2.440042 1.365203 2.502062 3.583473

7 C 4.253919 2.933843 2.375395 3.730380 4.639065

8 N 4.189831 2.837421 2.929710 4.396827 4.973717

9 C 5.526402 4.186729 4.251303 5.711345 6.336170

10 C 6.368541 5.005012 4.660157 6.019184 6.908133

11 C 5.729737 4.415530 3.753513 4.979451 6.023023

12 N 1.369655 2.440436 3.545911 3.596699 2.500670

13 C 3.768305 4.425931 5.733914 6.043032 4.982719

14 C 4.655646 4.988848 6.344483 6.906546 6.001624

15 C 4.267310 4.192722 5.522650 6.354559 5.707557

16 N 2.944374 2.837896 4.180577 4.988219 4.390618

17 C 2.376107 2.922139 4.236723 4.643052 3.719048

18 N 5.346546 5.009647 6.256389 7.273229 6.791161

19 N 4.942537 4.021535 4.928271 6.246726 6.235448

20 C 5.596412 4.928271 6.007027 7.217015 6.991175

21 C 7.015461 6.246726 7.217015 8.508369 8.384704

22 C 7.218811 6.235448 6.991175 8.384704 8.484945

23 C 6.034200 4.942537 5.596412 7.015461 7.218811

24 N 6.269566 5.010815 5.333510 6.799821 7.260952

25 Zn 3.017100 2.010768 3.003513 4.254185 4.242473

26 C 3.741279 3.720046 2.616761 1.488785 2.588684

27 H 2.247953 3.315676 3.330754 2.205664 1.081175

28 C 7.846257 6.481535 6.133005 7.466387 8.388433

29 H 6.334596 5.097513 4.200930 5.212335 6.402453

30 C 4.415864 5.379023 6.579229 6.580810 5.337524

31 H 5.724014 6.065261 7.421592 7.982067 7.049213

32 C 8.177913 7.544354 8.594440 9.831040 9.589865

33 H 8.221887 7.179108 7.835508 9.261649 9.448552

34 H 4.129527 4.427571 3.512464 2.142140 2.757315

35 H 4.322254 4.127498 2.936196 2.143560 3.298721

36 H 4.322254 4.127498 2.936196 2.143560 3.298721

37 H 8.251536 6.897497 6.654451 8.014090 8.872999

38 H 8.251536 6.897497 6.654451 8.014090 8.872999

39 H 8.392717 7.043038 6.501127 7.727229 8.772951

40 H 4.340662 5.406877 6.517966 6.379180 5.098083

41 H 4.340662 5.406877 6.517966 6.379180 5.098083

42 H 5.482767 6.385502 7.620379 7.666730 6.428463

43 H 8.271992 7.742872 8.850021 10.025132 9.696264

44 H 8.271992 7.742872 8.850021 10.025132 9.696264

45 H 9.108822 8.384559 9.355353 10.650129 10.498200

6 7 8 9 10

6 N 0.000000

7 C 1.321022 0.000000

8 N 2.414700 1.367509 0.000000

9 C 3.517296 2.233169 1.363266 0.000000

10 C 3.553833 2.292623 2.320216 1.503898 0.000000

11 C 2.479076 1.481700 2.304436 2.286332 1.349426

12 N 4.824091 5.357717 5.015570 6.263010 7.304887

13 C 6.847402 7.028265 6.259991 7.229949 8.550163

14 C 7.288163 7.225212 6.245555 7.003788 8.427979

15 C 6.270477 6.016640 4.924240 5.576214 7.028265

16 N 5.015124 4.924240 4.004558 4.913346 6.259991

17 C 5.345451 5.576214 4.913346 5.996869 7.229949

18 N 6.777020 6.270477 5.015124 5.345451 6.847402

19 N 5.009647 4.192722 2.837896 2.922139 4.425931

20 C 6.256389 5.522650 4.180577 4.236723 5.733914

21 C 7.273229 6.354559 4.988219 4.643052 6.043032

22 C 6.791161 5.707557 4.390618 3.719048 4.982719

23 C 5.346546 4.267310 2.944374 2.376107 3.768305

24 N 4.761279 3.517454 2.416595 1.316648 2.483726

25 Zn 3.388510 3.008320 2.002279 2.998435 4.275081

26 C 3.077636 4.398074 5.368753 6.575911 6.568643

27 H 4.604440 5.704977 6.051282 7.414256 7.981558

28 C 4.976806 3.758475 3.735472 2.632403 1.485296

29 H 2.837881 2.271154 3.333709 3.348781 2.186891

30 C 7.813656 8.175063 7.544688 8.597063 9.859227

31 H 8.342427 8.223594 7.182638 7.839168 9.298162

32 C 8.727073 7.837510 6.470269 6.116230 7.488339

33 H 7.497337 6.324567 5.084010 4.178152 5.224396

34 H 4.141427 5.461912 6.369256 7.612506 7.653945

35 H 3.085806 4.340681 5.414301 6.531911 6.379827

36 H 3.085806 4.340681 5.414301 6.531911 6.379827

37 H 5.567257 4.327172 4.127235 2.933172 2.135427

38 H 5.567257 4.327172 4.127235 2.933172 2.135427

39 H 5.231398 4.163075 4.455084 3.537630 2.140458

40 H 7.790575 8.252210 7.727068 8.837485 10.035736

41 H 7.790575 8.252210 7.727068 8.837485 10.035736

42 H 8.825481 9.113805 8.394231 9.367980 10.689422

43 H 9.074345 8.255932 6.899676 6.649609 8.046887

44 H 9.074345 8.255932 6.899676 6.649609 8.046887

45 H 9.361113 8.371699 7.019164 6.469067 7.732246

11 12 13 14 15

11 C 0.000000

12 N 6.836845 0.000000

13 C 8.427979 2.483726 0.000000

14 C 8.520463 3.540385 1.349426 0.000000

15 C 7.225212 3.517454 2.292623 1.481700 0.000000

16 N 6.245555 2.416595 2.320216 2.304436 1.367509

17 C 7.003788 1.316648 1.503898 2.286332 2.233169

18 N 7.288163 4.761279 3.553833 2.479076 1.321022

19 N 4.988848 5.010815 5.005012 4.415530 2.933843

20 C 6.344483 5.333510 4.660157 3.753513 2.375395

21 C 6.906546 6.799821 6.019184 4.979451 3.730380

22 C 6.001624 7.260952 6.908133 6.023023 4.639065

23 C 4.655646 6.269566 6.368541 5.729737 4.253919

24 N 3.540385 6.779031 7.304887 6.836845 5.357717

25 Zn 4.260231 3.389515 4.275081 4.260231 3.008320

26 C 5.348878 5.016639 7.488339 8.387985 7.837510

27 H 7.066632 2.865690 5.224396 6.388175 6.324567

28 C 2.571660 8.748947 9.859227 9.619955 8.175063

29 H 1.081234 7.537584 9.298162 9.477116 8.223594

30 C 9.619955 3.048176 1.485296 2.571660 3.758475

31 H 9.477116 4.565974 2.186891 1.081234 2.271154

32 C 8.387985 7.776928 6.568643 5.348878 4.398074

33 H 6.388175 8.319398 7.981558 7.066632 5.704977

34 H 6.440116 5.254967 7.732246 8.754536 8.371699

35 H 5.122316 5.616183 8.046887 8.886111 8.255932

36 H 5.122316 5.616183 8.046887 8.886111 8.255932

37 H 3.276106 9.078383 10.035736 9.710287 8.252210

38 H 3.276106 9.078383 10.035736 9.710287 8.252210

39 H 2.755007 9.399604 10.689422 10.535736 9.113805

40 H 9.710287 3.046964 2.135427 3.276106 4.327172

41 H 9.710287 3.046964 2.135427 3.276106 4.327172

42 H 10.535736 4.113116 2.140458 2.755007 4.163075

43 H 8.886111 7.767757 6.379827 5.122316 4.340681

44 H 8.886111 7.767757 6.379827 5.122316 4.340681

45 H 8.754536 8.785260 7.653945 6.440116 5.461912

16 17 18 19 20

16 N 0.000000

17 C 1.363266 0.000000

18 N 2.414700 3.517296 0.000000

19 N 2.837421 4.186729 2.440042 0.000000

20 C 2.929710 4.251303 1.365203 1.356725 0.000000

21 C 4.396827 5.711345 2.502062 2.293680 1.467328

22 C 4.973717 6.336170 3.583473 2.280944 2.272181

23 C 4.189831 5.526402 3.547425 1.365097 2.219942

24 N 5.015570 6.263010 4.824091 2.440436 3.545911

25 Zn 2.002279 2.998435 3.388510 2.010768 3.003513

26 C 6.470269 6.116230 8.727073 7.544354 8.594440

27 H 5.084010 4.178152 7.497337 7.179108 7.835508

28 C 7.544688 8.597063 7.813656 5.379023 6.579229

29 H 7.182638 7.839168 8.342427 6.065261 7.421592

30 C 3.735472 2.632403 4.976806 6.481535 6.133005

31 H 3.333709 3.348781 2.837881 5.097513 4.200930

32 C 5.368753 6.575911 3.077636 3.720046 2.616761

33 H 6.051282 7.414256 4.604440 3.315676 3.330754

34 H 7.019164 6.469067 9.361113 8.384559 9.355353

35 H 6.899676 6.649609 9.074345 7.742872 8.850021

36 H 6.899676 6.649609 9.074345 7.742872 8.850021

37 H 7.727068 8.837485 7.790575 5.406877 6.517966

38 H 7.727068 8.837485 7.790575 5.406877 6.517966

39 H 8.394231 9.367980 8.825481 6.385502 7.620379

40 H 4.127235 2.933172 5.567257 6.897497 6.654451

41 H 4.127235 2.933172 5.567257 6.897497 6.654451

42 H 4.455084 3.537630 5.231398 7.043038 6.501127

43 H 5.414301 6.531911 3.085806 4.127498 2.936196

44 H 5.414301 6.531911 3.085806 4.127498 2.936196

45 H 6.369256 7.612506 4.141427 4.427571 3.512464

21 22 23 24 25

21 C 0.000000

22 C 1.374793 0.000000

23 C 2.277119 1.446274 0.000000

24 N 3.596699 2.500670 1.369655 0.000000

25 Zn 4.254185 4.242473 3.017100 3.389515 0.000000

26 C 9.831040 9.589865 8.177913 7.776928 5.597752

27 H 9.261649 9.448552 8.221887 8.319398 5.217611

28 C 6.580810 5.337524 4.415864 3.048176 5.606149

29 H 7.982067 7.049213 5.724014 4.565974 5.229037

30 C 7.466387 8.388433 7.846257 8.748947 5.606149

31 H 5.212335 6.402453 6.334596 7.537584 5.229037

32 C 1.488785 2.588684 3.741279 5.016639 5.597752

33 H 2.205664 1.081175 2.247953 2.865690 5.217611

34 H 10.650129 10.498200 9.108822 8.785260 6.396008

35 H 10.025132 9.696264 8.271992 7.767757 5.869495

36 H 10.025132 9.696264 8.271992 7.767757 5.869495

37 H 6.379180 5.098083 4.340662 3.046964 5.861886

38 H 6.379180 5.098083 4.340662 3.046964 5.861886

39 H 7.666730 6.428463 5.482767 4.113116 6.414540

40 H 8.014090 8.872999 8.251536 9.078383 5.861886

41 H 8.014090 8.872999 8.251536 9.078383 5.861886

42 H 7.727229 8.772951 8.392717 9.399604 6.414540

43 H 2.143560 3.298721 4.322254 5.616183 5.869495

44 H 2.143560 3.298721 4.322254 5.616183 5.869495

45 H 2.142140 2.757315 4.129527 5.254967 6.396008

26 27 28 29 30

26 C 0.000000

27 H 2.989654 0.000000

28 C 7.919402 9.459578 0.000000

29 H 5.276575 7.390920 2.985222 0.000000

30 C 7.925310 5.274575 11.212299 10.422664 0.000000

31 H 9.461134 7.382878 10.422664 10.458074 2.985222

32 C 11.195503 10.400892 7.925310 9.461134 7.919402

33 H 10.400892 10.435222 5.274575 7.382878 9.459578

34 H 1.091361 2.739149 9.010382 6.352150 7.967978

35 H 1.095149 3.744638 7.663773 4.938359 8.545545

36 H 1.095149 3.744638 7.663773 4.938359 8.545545

37 H 8.531176 9.945704 1.094775 3.738168 11.418524

38 H 8.531176 9.945704 1.094775 3.738168 11.418524

39 H 7.979433 9.820747 1.090949 2.749839 11.998346

40 H 7.655853 4.924765 11.418524 10.461127 1.094775

41 H 7.655853 4.924765 11.418524 10.461127 1.094775

42 H 9.016149 6.347638 11.998346 11.376146 1.090949

43 H 11.418066 10.455934 8.545545 9.959930 7.663773

44 H 11.418066 10.455934 8.545545 9.959930 7.663773

45 H 11.970649 11.347327 7.967978 9.805799 9.010382

31 32 33 34 35

31 H 0.000000

32 C 5.276575 0.000000

33 H 7.390920 2.989654 0.000000

34 H 9.805799 11.970649 11.347327 0.000000

35 H 9.959930 11.418066 10.455934 1.771808 0.000000

36 H 9.959930 11.418066 10.455934 1.771808 1.754142

37 H 10.461127 7.655853 4.924765 9.615161 8.202509

38 H 10.461127 7.655853 4.924765 9.615161 8.387914

39 H 11.376146 9.016149 6.347638 9.065097 7.645758

40 H 3.738168 8.531176 9.945704 7.621676 8.201722

41 H 3.738168 8.531176 9.945704 7.621676 8.387145

42 H 2.749839 7.979433 9.820747 9.051769 9.630004

43 H 4.938359 1.095149 3.744638 12.148271 11.607190

44 H 4.938359 1.095149 3.744638 12.148271 11.738990

45 H 6.352150 1.091361 2.739149 12.792017 12.148271

36 37 38 39 40

36 H 0.000000

37 H 8.387914 0.000000

38 H 8.202509 1.753538 0.000000

39 H 7.645758 1.774836 1.774836 0.000000

40 H 8.387145 11.591890 11.723771 12.160017 0.000000

41 H 8.201722 11.723771 11.591890 12.160017 1.753538

42 H 9.630004 12.160017 12.160017 12.829080 1.774836

43 H 11.738990 8.201722 8.387145 9.630004 8.202509

44 H 11.607190 8.387145 8.201722 9.630004 8.387914

45 H 12.148271 7.621676 7.621676 9.051769 9.615161

41 42 43 44 45

41 H 0.000000

42 H 1.774836 0.000000

43 H 8.387914 7.645758 0.000000

44 H 8.202509 7.645758 1.754142 0.000000

45 H 9.615161 9.065097 1.771808 1.771808 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=0 Diff= 9.71D-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

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1 6 0 2.805729 -1.109404 0.000000

2 7 0 2.010768 0.000336 0.000000

3 6 0 2.790683 1.110487 0.000000

4 6 0 4.197362 0.692991 0.000000

5 6 0 4.187335 -0.681766 0.000000

6 7 0 2.379628 2.412337 0.000000

7 6 0 1.114963 2.794074 0.000000

8 7 0 0.000000 2.002279 0.000000

9 6 0 -1.118174 2.782139 0.000000

10 6 0 -0.679711 4.220701 0.000000

11 6 0 0.669649 4.207272 0.000000

12 7 0 2.381651 -2.411753 0.000000

13 6 0 0.679711 -4.220701 0.000000

14 6 0 -0.669649 -4.207272 0.000000

15 6 0 -1.114963 -2.794074 0.000000

16 7 0 -0.000000 -2.002279 0.000000

17 6 0 1.118174 -2.782139 0.000000

18 7 0 -2.379628 -2.412337 0.000000

19 7 0 -2.010768 -0.000336 0.000000

20 6 0 -2.790683 -1.110487 0.000000

21 6 0 -4.197362 -0.692991 0.000000

22 6 0 -4.187335 0.681766 0.000000

23 6 0 -2.805729 1.109404 0.000000

24 7 0 -2.381651 2.411753 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 5.355708 1.628254 0.000000

27 1 0 5.041321 -1.344824 0.000000

28 6 0 -1.626696 5.364958 0.000000

29 1 0 1.342268 5.053825 0.000000

30 6 0 1.626696 -5.364958 0.000000

31 1 0 -1.342268 -5.053825 0.000000

32 6 0 -5.355708 -1.628254 0.000000

33 1 0 -5.041321 1.344824 0.000000

34 1 0 6.303064 1.086418 0.000000

35 1 0 5.335370 2.283757 0.877071

36 1 0 5.335370 2.283757 -0.877071

37 1 0 -2.281257 5.328118 0.876769

38 1 0 -2.281257 5.328118 -0.876769

39 1 0 -1.098865 6.319717 0.000000

40 1 0 2.281257 -5.328118 0.876769

41 1 0 2.281257 -5.328118 -0.876769

42 1 0 1.098865 -6.319717 0.000000

43 1 0 -5.335370 -2.283757 0.877071

44 1 0 -5.335370 -2.283757 -0.877071

45 1 0 -6.303064 -1.086418 0.000000

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

Rotational constants (GHZ): 0.1829054 0.1818183 0.0913846

Leave Link 202 at Tue Sep 17 14:16:38 2019, MaxMem= 2415919104 cpu: 0.1

(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 101 beta electrons

nuclear repulsion energy 2761.2948354661 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= -0.1142066561 Hartrees.

Nuclear repulsion after empirical dispersion term = 2761.1806288100 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 = 3494

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.23D-06

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 130

GePol: Fraction of low-weight points (<1% of avg) = 3.72%

GePol: Cavity surface area = 382.158 Ang\*\*2

GePol: Cavity volume = 379.353 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0107135119 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2761.1699152980 Hartrees.

Leave Link 301 at Tue Sep 17 14:16:38 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= 15325 LenP2D= 41256.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.85D-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 14:16:39 2019, MaxMem= 2415919104 cpu: 14.6

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:16:39 2019, MaxMem= 2415919104 cpu: 1.7

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= -0.000000 -0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000342 Ang= 0.04 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 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0179 S= 1.0059

Leave Link 401 at Tue Sep 17 14:16:40 2019, MaxMem= 2415919104 cpu: 22.6

(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= 36624108.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.77D-15 for 3477.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.77D-15 for 2271 2141.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.99D-15 for 3477.

Iteration 1 A^-1\*A deviation from orthogonality is 1.62D-11 for 1981 1967.

E= -1275.84264764407

DIIS: error= 1.62D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.84264764407 IErMin= 1 ErrMin= 1.62D-04

ErrMax= 1.62D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.83D-05 BMatP= 6.83D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.62D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.303 Goal= None Shift= 0.000

Gap= 0.393 Goal= None Shift= 0.000

RMSDP=1.25D-05 MaxDP=3.06D-04 OVMax= 3.86D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.25D-05 CP: 1.00D+00

E= -1275.84267071678 Delta-E= -0.000023072708 Rises=F Damp=F

DIIS: error= 9.26D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84267071678 IErMin= 2 ErrMin= 9.26D-05

ErrMax= 9.26D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.58D-06 BMatP= 6.83D-05

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

Coeff-Com: 0.102D+00 0.898D+00

Coeff: 0.102D+00 0.898D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=5.92D-06 MaxDP=3.00D-04 DE=-2.31D-05 OVMax= 3.91D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 5.65D-06 CP: 1.00D+00 1.14D+00

E= -1275.84267081432 Delta-E= -0.000000097543 Rises=F Damp=F

DIIS: error= 1.40D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1275.84267081432 IErMin= 2 ErrMin= 9.26D-05

ErrMax= 1.40D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.42D-05 BMatP= 6.58D-06

IDIUse=3 WtCom= 4.58D-01 WtEn= 5.42D-01

Coeff-Com: -0.128D-01 0.609D+00 0.404D+00

Coeff-En: 0.000D+00 0.489D+00 0.511D+00

Coeff: -0.586D-02 0.544D+00 0.462D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.41D-06 MaxDP=1.89D-04 DE=-9.75D-08 OVMax= 6.73D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.84D-06 CP: 1.00D+00 1.23D+00 7.37D-01

E= -1275.84267394328 Delta-E= -0.000003128958 Rises=F Damp=F

DIIS: error= 6.25D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84267394328 IErMin= 4 ErrMin= 6.25D-05

ErrMax= 6.25D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.10D-06 BMatP= 6.58D-06

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

Coeff-Com: -0.985D-02 0.164D+00 0.237D+00 0.609D+00

Coeff: -0.985D-02 0.164D+00 0.237D+00 0.609D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.28D-06 MaxDP=1.26D-04 DE=-3.13D-06 OVMax= 1.64D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 9.78D-07 CP: 1.00D+00 1.28D+00 1.08D+00 1.12D+00

E= -1275.84267468935 Delta-E= -0.000000746078 Rises=F Damp=F

DIIS: error= 3.65D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84267468935 IErMin= 5 ErrMin= 3.65D-05

ErrMax= 3.65D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.79D-07 BMatP= 1.10D-06

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

Coeff-Com: 0.125D-03-0.501D-01-0.748D-02 0.369D+00 0.688D+00

Coeff: 0.125D-03-0.501D-01-0.748D-02 0.369D+00 0.688D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.10D-06 MaxDP=9.97D-05 DE=-7.46D-07 OVMax= 1.58D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 4.20D-07 CP: 1.00D+00 1.35D+00 1.31D+00 1.57D+00 1.26D+00

E= -1275.84267524015 Delta-E= -0.000000550795 Rises=F Damp=F

DIIS: error= 2.90D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84267524015 IErMin= 6 ErrMin= 2.90D-05

ErrMax= 2.90D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.80D-07 BMatP= 3.79D-07

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

Coeff-Com: 0.103D-01-0.154D+00-0.283D+00-0.342D+00 0.131D+00 0.164D+01

Coeff: 0.103D-01-0.154D+00-0.283D+00-0.342D+00 0.131D+00 0.164D+01

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.88D-06 MaxDP=2.52D-04 DE=-5.51D-07 OVMax= 3.76D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 4.37D-07 CP: 1.00D+00 1.51D+00 1.89D+00 2.50D+00 2.52D+00

CP: 2.52D+00

E= -1275.84267604688 Delta-E= -0.000000806735 Rises=F Damp=F

DIIS: error= 1.62D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84267604688 IErMin= 7 ErrMin= 1.62D-05

ErrMax= 1.62D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.04D-08 BMatP= 1.80D-07

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

Coeff-Com: 0.718D-02-0.781D-01-0.216D+00-0.415D+00-0.262D+00 0.117D+01

Coeff-Com: 0.796D+00

Coeff: 0.718D-02-0.781D-01-0.216D+00-0.415D+00-0.262D+00 0.117D+01

Coeff: 0.796D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.12D-06 MaxDP=1.56D-04 DE=-8.07D-07 OVMax= 2.38D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 6.12D-07 CP: 1.00D+00 1.61D+00 2.26D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.32D+00

E= -1275.84267627367 Delta-E= -0.000000226783 Rises=F Damp=F

DIIS: error= 5.31D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84267627367 IErMin= 8 ErrMin= 5.31D-06

ErrMax= 5.31D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.26D-08 BMatP= 9.04D-08

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

Coeff-Com: -0.780D-03 0.420D-01 0.180D-01-0.312D-01-0.169D+00-0.123D+00

Coeff-Com: 0.440D+00 0.824D+00

Coeff: -0.780D-03 0.420D-01 0.180D-01-0.312D-01-0.169D+00-0.123D+00

Coeff: 0.440D+00 0.824D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=8.35D-07 MaxDP=4.60D-05 DE=-2.27D-07 OVMax= 6.34D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 3.14D-07 CP: 1.00D+00 1.63D+00 2.35D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.68D+00 1.78D+00

E= -1275.84267630059 Delta-E= -0.000000026919 Rises=F Damp=F

DIIS: error= 2.85D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84267630059 IErMin= 9 ErrMin= 2.85D-06

ErrMax= 2.85D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.44D-09 BMatP= 2.26D-08

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

Coeff-Com: -0.211D-02 0.409D-01 0.582D-01 0.781D-01-0.211D-01-0.346D+00

Coeff-Com: 0.375D-01 0.448D+00 0.706D+00

Coeff: -0.211D-02 0.409D-01 0.582D-01 0.781D-01-0.211D-01-0.346D+00

Coeff: 0.375D-01 0.448D+00 0.706D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.08D-07 MaxDP=1.79D-05 DE=-2.69D-08 OVMax= 2.21D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 7.99D-08 CP: 1.00D+00 1.64D+00 2.38D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.83D+00 2.10D+00 1.16D+00

E= -1275.84267630617 Delta-E= -0.000000005588 Rises=F Damp=F

DIIS: error= 1.33D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84267630617 IErMin=10 ErrMin= 1.33D-06

ErrMax= 1.33D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.32D-09 BMatP= 6.44D-09

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

Coeff-Com: -0.667D-03 0.644D-02 0.207D-01 0.476D-01 0.473D-01-0.125D+00

Coeff-Com: -0.115D+00-0.117D-01 0.319D+00 0.811D+00

Coeff: -0.667D-03 0.644D-02 0.207D-01 0.476D-01 0.473D-01-0.125D+00

Coeff: -0.115D+00-0.117D-01 0.319D+00 0.811D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=8.26D-08 MaxDP=4.75D-06 DE=-5.59D-09 OVMax= 3.54D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 6.03D-08 CP: 1.00D+00 1.64D+00 2.39D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.89D+00 2.16D+00 1.18D+00 1.07D+00

E= -1275.84267630738 Delta-E= -0.000000001205 Rises=F Damp=F

DIIS: error= 7.48D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84267630738 IErMin=11 ErrMin= 7.48D-07

ErrMax= 7.48D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.44D-10 BMatP= 1.32D-09

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

Coeff-Com: 0.134D-03-0.654D-02-0.392D-02 0.603D-02 0.263D-01 0.180D-01

Coeff-Com: -0.696D-01-0.952D-01-0.215D-01 0.418D+00 0.728D+00

Coeff: 0.134D-03-0.654D-02-0.392D-02 0.603D-02 0.263D-01 0.180D-01

Coeff: -0.696D-01-0.952D-01-0.215D-01 0.418D+00 0.728D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=7.20D-08 MaxDP=4.01D-06 DE=-1.21D-09 OVMax= 4.91D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 2.29D-08 CP: 1.00D+00 1.64D+00 2.39D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.92D+00 2.22D+00 1.24D+00 1.32D+00

CP: 1.20D+00

E= -1275.84267630784 Delta-E= -0.000000000465 Rises=F Damp=F

DIIS: error= 4.89D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84267630784 IErMin=12 ErrMin= 4.89D-07

ErrMax= 4.89D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.62D-10 BMatP= 4.44D-10

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

Coeff-Com: 0.291D-03-0.591D-02-0.934D-02-0.111D-01-0.166D-02 0.515D-01

Coeff-Com: -0.723D-02-0.444D-01-0.130D+00-0.211D-01 0.406D+00 0.772D+00

Coeff: 0.291D-03-0.591D-02-0.934D-02-0.111D-01-0.166D-02 0.515D-01

Coeff: -0.723D-02-0.444D-01-0.130D+00-0.211D-01 0.406D+00 0.772D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=5.95D-08 MaxDP=2.89D-06 DE=-4.65D-10 OVMax= 4.28D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.43D-08 CP: 1.00D+00 1.64D+00 2.40D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.94D+00 2.28D+00 1.30D+00 1.48D+00

CP: 1.40D+00 1.26D+00

E= -1275.84267630805 Delta-E= -0.000000000211 Rises=F Damp=F

DIIS: error= 2.07D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84267630805 IErMin=13 ErrMin= 2.07D-07

ErrMax= 2.07D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.72D-11 BMatP= 1.62D-10

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

Coeff-Com: 0.106D-03-0.640D-03-0.327D-02-0.671D-02-0.102D-01 0.191D-01

Coeff-Com: 0.158D-01 0.131D-01-0.603D-01-0.149D+00-0.281D-01 0.368D+00

Coeff-Com: 0.842D+00

Coeff: 0.106D-03-0.640D-03-0.327D-02-0.671D-02-0.102D-01 0.191D-01

Coeff: 0.158D-01 0.131D-01-0.603D-01-0.149D+00-0.281D-01 0.368D+00

Coeff: 0.842D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.68D-08 MaxDP=1.74D-06 DE=-2.11D-10 OVMax= 2.63D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 7.43D-09 CP: 1.00D+00 1.64D+00 2.40D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.95D+00 2.31D+00 1.33D+00 1.58D+00

CP: 1.51D+00 1.56D+00 1.38D+00

E= -1275.84267630813 Delta-E= -0.000000000073 Rises=F Damp=F

DIIS: error= 8.20D-08 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84267630813 IErMin=14 ErrMin= 8.20D-08

ErrMax= 8.20D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.06D-11 BMatP= 3.72D-11

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

Coeff-Com: -0.157D-04 0.122D-02 0.520D-03-0.108D-02-0.584D-02-0.195D-02

Coeff-Com: 0.111D-01 0.206D-01-0.132D-02-0.841D-01-0.115D+00 0.555D-02

Coeff-Com: 0.465D+00 0.706D+00

Coeff: -0.157D-04 0.122D-02 0.520D-03-0.108D-02-0.584D-02-0.195D-02

Coeff: 0.111D-01 0.206D-01-0.132D-02-0.841D-01-0.115D+00 0.555D-02

Coeff: 0.465D+00 0.706D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.12D-08 MaxDP=5.76D-07 DE=-7.28D-11 OVMax= 7.12D-06

Cycle 15 Pass 1 IDiag 1:

RMSU= 2.77D-09 CP: 1.00D+00 1.64D+00 2.41D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.95D+00 2.32D+00 1.34D+00 1.61D+00

CP: 1.56D+00 1.70D+00 1.62D+00 1.07D+00

E= -1275.84267630812 Delta-E= 0.000000000011 Rises=F Damp=F

DIIS: error= 3.67D-08 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=14 EnMin= -1275.84267630813 IErMin=15 ErrMin= 3.67D-08

ErrMax= 3.67D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.10D-12 BMatP= 1.06D-11

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

Coeff-Com: -0.293D-04 0.722D-03 0.954D-03 0.833D-03-0.616D-03-0.481D-02

Coeff-Com: 0.206D-02 0.685D-02 0.118D-01-0.131D-01-0.465D-01-0.719D-01

Coeff-Com: 0.525D-01 0.352D+00 0.709D+00

Coeff: -0.293D-04 0.722D-03 0.954D-03 0.833D-03-0.616D-03-0.481D-02

Coeff: 0.206D-02 0.685D-02 0.118D-01-0.131D-01-0.465D-01-0.719D-01

Coeff: 0.525D-01 0.352D+00 0.709D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.58D-09 MaxDP=1.86D-07 DE= 1.09D-11 OVMax= 1.03D-06

Error on total polarization charges = 0.06464

SCF Done: E(UB3LYP) = -1275.84267631 A.U. after 15 cycles

NFock= 15 Conv=0.26D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0177 S= 1.0059

<L.S>= 0.000000000000E+00

KE= 1.320799349713D+03 PE=-8.574286675772D+03 EE= 3.216474734452D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.72

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0177, after 2.0002

Leave Link 502 at Tue Sep 17 14:17:57 2019, MaxMem= 2415919104 cpu: 1353.0

(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= 15325 LenP2D= 41256.

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 = 244

Leave Link 701 at Tue Sep 17 14:18:01 2019, MaxMem= 2415919104 cpu: 69.5

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 14:18:01 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 14:18:11 2019, MaxMem= 2415919104 cpu: 176.3

(Enter /home/blab/g09/l716.exe)

Dipole = 9.05941988D-14-2.18047802D-13 2.22044605D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000519298 0.000109863 0.000000000

2 7 0.000390540 -0.000044597 0.000000000

3 6 0.000009297 0.000279841 0.000000000

4 6 -0.000080679 -0.000081091 -0.000000000

5 6 0.000005424 -0.000021938 0.000000000

6 7 -0.000223653 -0.000295408 0.000000000

7 6 0.000088033 0.000368213 0.000000000

8 7 -0.000230194 -0.000207433 -0.000000000

9 6 0.000277726 -0.000134492 -0.000000000

10 6 -0.000032444 0.000116215 -0.000000000

11 6 -0.000020207 -0.000041223 0.000000000

12 7 0.000284486 -0.000354078 0.000000000

13 6 0.000032444 -0.000116215 0.000000000

14 6 0.000020207 0.000041223 0.000000000

15 6 -0.000088033 -0.000368213 -0.000000000

16 7 0.000230194 0.000207433 -0.000000000

17 6 -0.000277726 0.000134492 0.000000000

18 7 0.000223653 0.000295408 -0.000000000

19 7 -0.000390540 0.000044597 0.000000000

20 6 -0.000009297 -0.000279841 -0.000000000

21 6 0.000080679 0.000081091 -0.000000000

22 6 -0.000005424 0.000021938 -0.000000000

23 6 0.000519298 -0.000109863 0.000000000

24 7 -0.000284486 0.000354078 0.000000000

25 30 0.000000000 -0.000000000 0.000000000

26 6 0.000029520 0.000002426 -0.000000000

27 1 0.000014451 0.000016064 -0.000000000

28 6 0.000032159 0.000043204 0.000000000

29 1 0.000004008 -0.000006945 0.000000000

30 6 -0.000032159 -0.000043204 -0.000000000

31 1 -0.000004008 0.000006945 0.000000000

32 6 -0.000029520 -0.000002426 0.000000000

33 1 -0.000014451 -0.000016064 -0.000000000

34 1 0.000000423 -0.000002114 0.000000000

35 1 -0.000006055 0.000011262 0.000000854

36 1 -0.000006055 0.000011262 -0.000000854

37 1 -0.000009320 -0.000015725 -0.000002456

38 1 -0.000009320 -0.000015725 0.000002456

39 1 -0.000001946 -0.000001236 0.000000000

40 1 0.000009320 0.000015725 -0.000002456

41 1 0.000009320 0.000015725 0.000002456

42 1 0.000001946 0.000001236 -0.000000000

43 1 0.000006055 -0.000011262 0.000000854

44 1 0.000006055 -0.000011262 -0.000000854

45 1 -0.000000423 0.000002114 -0.000000000

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

Cartesian Forces: Max 0.000519298 RMS 0.000134902

Leave Link 716 at Tue Sep 17 14:18:11 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 0.000328242 RMS 0.000055240

Search for a local minimum.

Step number 16 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 12 13 14 15

16

DE= -5.52D-06 DEPred=-2.45D-06 R= 2.25D+00

TightC=F SS= 1.41D+00 RLast= 1.45D-02 DXNew= 2.6636D-01 4.3441D-02

Trust test= 2.25D+00 RLast= 1.45D-02 DXMaxT set to 1.58D-01

ITU= 1 1 -1 1 1 1 -1 0 1 -1 1 1 1 1 0 0

Eigenvalues --- 0.00057 0.00878 0.00878 0.00878 0.00878

Eigenvalues --- 0.01336 0.01338 0.01346 0.01347 0.01604

Eigenvalues --- 0.01623 0.01631 0.01640 0.01774 0.01793

Eigenvalues --- 0.01809 0.01823 0.01890 0.01910 0.01939

Eigenvalues --- 0.01950 0.01997 0.02000 0.02045 0.02047

Eigenvalues --- 0.02070 0.02087 0.02103 0.02110 0.02115

Eigenvalues --- 0.02205 0.02312 0.02316 0.02351 0.02372

Eigenvalues --- 0.07117 0.07197 0.07197 0.07197 0.07197

Eigenvalues --- 0.07311 0.07352 0.07391 0.12815 0.13567

Eigenvalues --- 0.14498 0.14499 0.14531 0.15662 0.15976

Eigenvalues --- 0.15998 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16075 0.16234 0.17899 0.18522

Eigenvalues --- 0.22062 0.22094 0.23327 0.23841 0.23854

Eigenvalues --- 0.23885 0.24003 0.24910 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25037

Eigenvalues --- 0.25547 0.28547 0.29956 0.32633 0.32917

Eigenvalues --- 0.33190 0.33198 0.33282 0.33282 0.33417

Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33729 0.33875 0.34421 0.34437

Eigenvalues --- 0.34437 0.34437 0.35046 0.35443 0.35554

Eigenvalues --- 0.35564 0.35673 0.35682 0.35682 0.36221

Eigenvalues --- 0.38255 0.41024 0.41639 0.41818 0.43226

Eigenvalues --- 0.47715 0.48968 0.48981 0.49108 0.50639

Eigenvalues --- 0.51358 0.51361 0.52626 0.53932 0.54019

Eigenvalues --- 0.54025 0.56322 0.56328 0.57024

Cosine: 0.472 < 0.500

Cut down GDIIS temporarily because of the cosine check. E 6

DIIS coeff's: 1.15185 -0.39795 0.03821 0.02853 -0.00617

DIIS coeff's: 0.35374 -0.16821

Cosine: 0.512 > 0.500

Length: 0.550

GDIIS step was calculated using 7 of the last 16 vectors.

Iteration 1 RMS(Cart)= 0.00052259 RMS(Int)= 0.00000384

Iteration 2 RMS(Cart)= 0.00000071 RMS(Int)= 0.00000383

ITry= 1 IFail=0 DXMaxC= 2.25D-03 DCOld= 1.00D+10 DXMaxT= 1.58D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 4.19D-11 for atom 39.

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

(Linear) (Quad) (Total)

R1 2.57966 0.00027 0.00211 0.00089 0.00299 2.58265

R2 2.73306 -0.00002 -0.00054 -0.00115 -0.00169 2.73137

R3 2.58827 -0.00033 -0.00090 -0.00007 -0.00097 2.58730

R4 2.56384 -0.00018 -0.00159 -0.00121 -0.00280 2.56103

R5 3.79980 -0.00002 -0.00070 0.00049 -0.00023 3.79957

R6 2.77285 0.00009 0.00116 -0.00052 0.00065 2.77349

R7 2.57986 -0.00007 0.00051 0.00054 0.00106 2.58092

R8 2.59798 -0.00002 0.00000 0.00030 0.00031 2.59829

R9 2.81340 -0.00002 -0.00023 0.00003 -0.00020 2.81320

R10 2.04312 -0.00002 -0.00006 -0.00008 -0.00014 2.04298

R11 2.49637 0.00027 0.00093 -0.00006 0.00088 2.49725

R12 2.58422 -0.00014 -0.00144 -0.00081 -0.00225 2.58197

R13 2.80001 0.00004 0.00077 0.00047 0.00124 2.80125

R14 2.57620 0.00020 0.00186 0.00077 0.00262 2.57882

R15 3.78376 -0.00008 -0.00101 0.00012 -0.00089 3.78287

R16 2.84196 -0.00010 -0.00072 -0.00005 -0.00077 2.84118

R17 2.48810 0.00015 -0.00028 -0.00076 -0.00103 2.48707

R18 2.55005 0.00007 -0.00024 -0.00016 -0.00040 2.54965

R19 2.80680 0.00001 0.00011 -0.00011 -0.00000 2.80680

R20 2.04324 0.00001 -0.00010 0.00022 0.00013 2.04336

R21 2.48810 0.00015 -0.00028 -0.00076 -0.00103 2.48707

R22 2.55005 0.00007 -0.00024 -0.00016 -0.00040 2.54965

R23 2.84196 -0.00010 -0.00072 -0.00005 -0.00077 2.84118

R24 2.80680 0.00001 0.00011 -0.00011 -0.00000 2.80680

R25 2.80001 0.00004 0.00077 0.00047 0.00124 2.80125

R26 2.04324 0.00001 -0.00010 0.00022 0.00013 2.04336

R27 2.58422 -0.00014 -0.00144 -0.00081 -0.00225 2.58197

R28 2.49637 0.00027 0.00093 -0.00006 0.00088 2.49725

R29 2.57620 0.00020 0.00186 0.00077 0.00262 2.57882

R30 3.78376 -0.00008 -0.00101 0.00012 -0.00089 3.78287

R31 2.57986 -0.00007 0.00051 0.00054 0.00106 2.58092

R32 2.56384 -0.00018 -0.00159 -0.00121 -0.00280 2.56103

R33 2.57966 0.00027 0.00211 0.00089 0.00299 2.58265

R34 3.79980 -0.00002 -0.00070 0.00049 -0.00023 3.79957

R35 2.77285 0.00009 0.00116 -0.00052 0.00065 2.77349

R36 2.59798 -0.00002 0.00000 0.00030 0.00031 2.59829

R37 2.81340 -0.00002 -0.00023 0.00003 -0.00020 2.81320

R38 2.73306 -0.00002 -0.00054 -0.00115 -0.00169 2.73137

R39 2.04312 -0.00002 -0.00006 -0.00008 -0.00014 2.04298

R40 2.58827 -0.00033 -0.00090 -0.00007 -0.00097 2.58730

R41 2.06237 0.00000 -0.00006 0.00007 0.00001 2.06238

R42 2.06953 -0.00001 -0.00015 0.00015 0.00000 2.06954

R43 2.06953 -0.00001 -0.00015 0.00015 0.00000 2.06954

R44 2.06882 -0.00001 -0.00020 0.00008 -0.00012 2.06870

R45 2.06882 -0.00001 -0.00020 0.00008 -0.00012 2.06870

R46 2.06159 0.00000 -0.00008 0.00003 -0.00005 2.06155

R47 2.06882 -0.00001 -0.00020 0.00008 -0.00012 2.06870

R48 2.06882 -0.00001 -0.00020 0.00008 -0.00012 2.06870

R49 2.06159 0.00000 -0.00008 0.00003 -0.00005 2.06155

R50 2.06953 -0.00001 -0.00015 0.00015 0.00000 2.06954

R51 2.06953 -0.00001 -0.00015 0.00015 0.00000 2.06954

R52 2.06237 0.00000 -0.00006 0.00007 0.00001 2.06238

A1 1.89224 -0.00001 0.00026 -0.00057 -0.00032 1.89192

A2 2.20518 0.00000 -0.00048 -0.00027 -0.00075 2.20443

A3 2.18576 0.00001 0.00022 0.00084 0.00108 2.18684

A4 1.90756 -0.00004 -0.00048 0.00029 -0.00019 1.90736

A5 2.19224 0.00001 -0.00037 -0.00057 -0.00094 2.19131

A6 2.18339 0.00003 0.00085 0.00028 0.00113 2.18452

A7 1.89470 0.00004 0.00042 0.00014 0.00056 1.89526

A8 2.22333 0.00004 0.00031 0.00023 0.00054 2.22387

A9 2.16515 -0.00008 -0.00073 -0.00037 -0.00110 2.16405

A10 1.85202 0.00003 -0.00004 -0.00026 -0.00030 1.85172

A11 2.17383 -0.00005 -0.00022 -0.00014 -0.00037 2.17346

A12 2.25733 0.00003 0.00027 0.00041 0.00067 2.25801

A13 1.87826 -0.00002 -0.00015 0.00040 0.00025 1.87851

A14 2.18122 0.00000 0.00009 -0.00020 -0.00011 2.18111

A15 2.22370 0.00002 0.00006 -0.00021 -0.00015 2.22356

A16 2.16979 -0.00007 -0.00155 -0.00061 -0.00215 2.16764

A17 2.23093 -0.00001 0.00035 0.00029 0.00064 2.23158

A18 2.16921 -0.00000 -0.00061 -0.00051 -0.00112 2.16809

A19 1.88304 0.00001 0.00026 0.00022 0.00048 1.88352

A20 1.91508 -0.00001 -0.00034 0.00005 -0.00029 1.91479

A21 2.18830 0.00001 0.00078 0.00030 0.00108 2.18938

A22 2.17980 -0.00000 -0.00044 -0.00035 -0.00079 2.17902

A23 1.88395 0.00001 0.00007 -0.00030 -0.00023 1.88373

A24 2.24743 -0.00004 -0.00035 -0.00024 -0.00059 2.24684

A25 2.15180 0.00003 0.00027 0.00053 0.00081 2.15262

A26 1.85669 -0.00003 -0.00002 0.00028 0.00026 1.85695

A27 2.15440 0.00001 0.00014 -0.00024 -0.00010 2.15430

A28 2.27209 0.00002 -0.00012 -0.00004 -0.00016 2.27193

A29 1.88601 0.00002 0.00003 -0.00025 -0.00021 1.88579

A30 2.16493 -0.00001 -0.00008 0.00003 -0.00005 2.16488

A31 2.23225 -0.00001 0.00005 0.00022 0.00026 2.23251

A32 2.17075 0.00003 0.00089 0.00094 0.00182 2.17257

A33 1.85669 -0.00003 -0.00002 0.00028 0.00026 1.85695

A34 2.27209 0.00002 -0.00012 -0.00004 -0.00016 2.27193

A35 2.15440 0.00001 0.00014 -0.00024 -0.00010 2.15430

A36 1.88601 0.00002 0.00003 -0.00025 -0.00021 1.88579

A37 2.23225 -0.00001 0.00005 0.00022 0.00026 2.23251

A38 2.16493 -0.00001 -0.00008 0.00003 -0.00005 2.16488

A39 1.88304 0.00001 0.00026 0.00022 0.00048 1.88352

A40 2.16921 -0.00000 -0.00061 -0.00051 -0.00112 2.16809

A41 2.23093 -0.00001 0.00035 0.00029 0.00064 2.23158

A42 1.91508 -0.00001 -0.00034 0.00005 -0.00029 1.91479

A43 2.18830 0.00001 0.00078 0.00030 0.00108 2.18938

A44 2.17980 -0.00000 -0.00044 -0.00035 -0.00079 2.17902

A45 2.15180 0.00003 0.00027 0.00053 0.00081 2.15262

A46 2.24743 -0.00004 -0.00035 -0.00024 -0.00059 2.24684

A47 1.88395 0.00001 0.00007 -0.00030 -0.00023 1.88373

A48 2.16979 -0.00007 -0.00155 -0.00061 -0.00215 2.16764

A49 1.90756 -0.00004 -0.00048 0.00029 -0.00019 1.90736

A50 2.18339 0.00003 0.00085 0.00028 0.00113 2.18452

A51 2.19224 0.00001 -0.00037 -0.00057 -0.00094 2.19131

A52 2.22333 0.00004 0.00031 0.00023 0.00054 2.22387

A53 2.16515 -0.00008 -0.00073 -0.00037 -0.00110 2.16405

A54 1.89470 0.00004 0.00042 0.00014 0.00056 1.89526

A55 1.85202 0.00003 -0.00004 -0.00026 -0.00030 1.85172

A56 2.17383 -0.00005 -0.00022 -0.00014 -0.00037 2.17346

A57 2.25733 0.00003 0.00027 0.00041 0.00067 2.25801

A58 1.87826 -0.00002 -0.00015 0.00040 0.00025 1.87851

A59 2.22370 0.00002 0.00006 -0.00021 -0.00015 2.22356

A60 2.18122 0.00000 0.00009 -0.00020 -0.00011 2.18111

A61 1.89224 -0.00001 0.00026 -0.00057 -0.00032 1.89192

A62 2.20518 0.00000 -0.00048 -0.00027 -0.00075 2.20443

A63 2.18576 0.00001 0.00022 0.00084 0.00108 2.18684

A64 2.17075 0.00003 0.00089 0.00094 0.00182 2.17257

A65 1.57063 -0.00000 -0.00075 -0.00049 -0.00125 1.56938

A66 1.57096 0.00000 0.00075 0.00049 0.00125 1.57221

A67 1.57096 0.00000 0.00075 0.00049 0.00125 1.57221

A68 1.57063 -0.00000 -0.00075 -0.00049 -0.00125 1.56938

A69 1.94281 0.00001 0.00032 -0.00014 0.00018 1.94300

A70 1.94074 -0.00001 -0.00015 0.00011 -0.00005 1.94069

A71 1.94074 -0.00001 -0.00015 0.00011 -0.00005 1.94069

A72 1.88945 0.00000 0.00004 -0.00001 0.00004 1.88949

A73 1.88945 0.00000 0.00004 -0.00001 0.00004 1.88949

A74 1.85749 0.00001 -0.00011 -0.00006 -0.00019 1.85730

A75 1.93401 -0.00001 -0.00014 0.00010 -0.00004 1.93397

A76 1.93401 -0.00001 -0.00014 0.00010 -0.00004 1.93397

A77 1.94523 -0.00000 0.00014 -0.00044 -0.00031 1.94492

A78 1.85748 0.00002 0.00008 0.00018 0.00027 1.85775

A79 1.89518 0.00000 0.00003 0.00005 0.00008 1.89526

A80 1.89518 0.00000 0.00003 0.00005 0.00008 1.89526

A81 1.93401 -0.00001 -0.00014 0.00010 -0.00004 1.93397

A82 1.93401 -0.00001 -0.00014 0.00010 -0.00004 1.93397

A83 1.94523 -0.00000 0.00014 -0.00044 -0.00031 1.94492

A84 1.85748 0.00002 0.00008 0.00018 0.00027 1.85775

A85 1.89518 0.00000 0.00003 0.00005 0.00008 1.89526

A86 1.89518 0.00000 0.00003 0.00005 0.00008 1.89526

A87 1.94074 -0.00001 -0.00015 0.00011 -0.00005 1.94069

A88 1.94074 -0.00001 -0.00015 0.00011 -0.00005 1.94069

A89 1.94281 0.00001 0.00032 -0.00014 0.00018 1.94300

A90 1.85749 0.00001 -0.00011 -0.00006 -0.00019 1.85730

A91 1.88945 0.00000 0.00004 -0.00001 0.00004 1.88949

A92 1.88945 0.00000 0.00004 -0.00001 0.00004 1.88949

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 1.03328 -0.00000 -0.00019 0.00003 -0.00015 1.03313

D31 -1.03328 0.00000 0.00019 -0.00003 0.00015 -1.03313

D32 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.10832 -0.00000 -0.00019 0.00003 -0.00015 -2.10846

D34 2.10832 0.00000 0.00019 -0.00003 0.00015 2.10846

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 1.02896 0.00000 -0.00004 0.00017 0.00014 1.02909

D64 -1.02896 -0.00000 0.00004 -0.00017 -0.00014 -1.02909

D65 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D66 -2.11264 0.00000 -0.00004 0.00017 0.00014 -2.11250

D67 2.11264 -0.00000 0.00004 -0.00017 -0.00014 2.11250

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 -2.11264 0.00000 -0.00004 0.00017 0.00014 -2.11250

D80 2.11264 -0.00000 0.00004 -0.00017 -0.00014 2.11250

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 1.02896 0.00000 -0.00004 0.00017 0.00014 1.02909

D83 -1.02896 -0.00000 0.00004 -0.00017 -0.00014 -1.02909

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 1.03328 -0.00000 -0.00019 0.00003 -0.00015 1.03313

D126 -1.03328 0.00000 0.00019 -0.00003 0.00015 -1.03313

D127 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D128 -2.10832 -0.00000 -0.00019 0.00003 -0.00015 -2.10846

D129 2.10832 0.00000 0.00019 -0.00003 0.00015 2.10846

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 0.000328 0.000450 YES

RMS Force 0.000055 0.000300 YES

Maximum Displacement 0.002251 0.001800 NO

RMS Displacement 0.000523 0.001200 YES

Predicted change in Energy=-2.964848D-06

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:18:11 2019, MaxMem= 2415919104 cpu: 1.5

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.073371 -2.192531 0.000000

2 7 0 -0.745993 -1.867137 0.000000

3 6 0 -0.006729 -3.002991 0.000000

4 6 0 -0.917397 -4.153963 0.000000

5 6 0 -2.189921 -3.633203 0.000000

6 7 0 1.355080 -3.106834 0.000000

7 6 0 2.178757 -2.073446 0.000000

8 7 0 1.857875 -0.745340 0.000000

9 6 0 2.998567 0.003727 0.000000

10 6 0 4.170647 -0.937925 0.000000

11 6 0 3.656872 -2.185490 0.000000

12 7 0 -3.123396 -1.313896 0.000000

13 6 0 -4.170647 0.937925 0.000000

14 6 0 -3.656872 2.185490 0.000000

15 6 0 -2.178757 2.073446 0.000000

16 7 0 -1.857875 0.745340 0.000000

17 6 0 -2.998567 -0.003727 0.000000

18 7 0 -1.355080 3.106834 0.000000

19 7 0 0.745993 1.867137 0.000000

20 6 0 0.006729 3.002991 0.000000

21 6 0 0.917397 4.153963 0.000000

22 6 0 2.189921 3.633203 0.000000

23 6 0 2.073371 2.192531 0.000000

24 7 0 3.123396 1.313896 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.479215 -5.576694 0.000000

27 1 0 -3.122925 -4.179356 0.000000

28 6 0 5.584926 -0.484140 0.000000

29 1 0 4.192673 -3.124708 0.000000

30 6 0 -5.584926 0.484140 0.000000

31 1 0 -4.192673 3.124708 0.000000

32 6 0 0.479215 5.576694 0.000000

33 1 0 3.122925 4.179356 0.000000

34 1 0 -1.333993 -6.255246 0.000000

35 1 0 0.137084 -5.801154 0.877011

36 1 0 0.137084 -5.801154 -0.877011

37 1 0 5.794020 0.137056 0.876805

38 1 0 5.794020 0.137056 -0.876805

39 1 0 6.274792 -1.329243 0.000000

40 1 0 -5.794020 -0.137056 0.876805

41 1 0 -5.794020 -0.137056 -0.876805

42 1 0 -6.274792 1.329243 0.000000

43 1 0 -0.137084 5.801154 0.877011

44 1 0 -0.137084 5.801154 -0.877011

45 1 0 1.333993 6.255246 0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.366680 0.000000

3 C 2.219878 1.355241 0.000000

4 C 2.276728 2.293241 1.467670 0.000000

5 C 1.445379 2.281210 2.272333 1.374957 0.000000

6 N 3.548271 2.439540 1.365762 2.502125 3.583866

7 C 4.253796 2.932018 2.374953 3.730244 4.638770

8 N 4.189160 2.835235 2.928094 4.395548 4.972364

9 C 5.527034 4.185912 4.251136 5.711494 6.336219

10 C 6.368815 5.003677 4.659932 6.019227 6.908064

11 C 5.730248 4.414360 3.753702 4.979842 6.023360

12 N 1.369143 2.440926 3.544948 3.596167 2.500113

13 C 3.768066 4.426808 5.733153 6.042430 4.981816

14 C 4.655593 4.989690 6.343807 6.906041 6.000762

15 C 4.267279 4.192971 5.521587 6.353869 5.706660

16 N 2.945764 2.839245 4.180518 4.988754 4.391116

17 C 2.376310 2.923420 4.236353 4.642815 3.718468

18 N 5.347823 5.011124 6.256837 7.273977 6.791543

19 N 4.942643 4.021296 4.927954 6.246640 6.234848

20 C 5.596451 4.927954 6.005997 7.216370 6.990303

21 C 7.015888 6.246640 7.216370 8.508120 8.384234

22 C 7.219061 6.234848 6.990303 8.384234 8.484319

23 C 6.035250 4.942643 5.596451 7.015888 7.219061

24 N 6.269085 5.009106 5.332278 6.798933 7.259829

25 Zn 3.017625 2.010648 3.002999 4.254060 4.242160

26 C 3.740841 3.719138 2.616714 1.488680 2.589145

27 H 2.247005 3.316046 3.330842 2.205674 1.081101

28 C 7.846535 6.480217 6.132797 7.466445 8.388375

29 H 6.335003 5.096264 4.201165 5.212694 6.402817

30 C 4.415380 5.379941 6.578478 6.580108 5.336532

31 H 5.724026 6.066145 7.420972 7.981635 7.048431

32 C 8.177809 7.543988 8.593436 9.830372 9.588873

33 H 8.222070 7.178342 7.834592 9.261123 9.447878

34 H 4.129447 4.427329 3.512661 2.142181 2.758209

35 H 4.321738 4.126193 2.935907 2.143436 3.299108

36 H 4.321738 4.126193 2.935907 2.143436 3.299108

37 H 8.251764 6.896183 6.654124 8.014034 8.872821

38 H 8.251764 6.896183 6.654124 8.014034 8.872821

39 H 8.392681 7.041360 6.500687 7.727006 8.772662

40 H 4.340160 5.407822 6.517293 6.378540 5.097191

41 H 4.340160 5.407822 6.517293 6.378540 5.097191

42 H 5.482228 6.386271 7.619506 7.665979 6.427444

43 H 8.271479 7.742261 8.848679 10.024091 9.694864

44 H 8.271479 7.742261 8.848679 10.024091 9.694864

45 H 9.109065 8.384476 9.354810 10.649901 10.497589

6 7 8 9 10

6 N 0.000000

7 C 1.321490 0.000000

8 N 2.414426 1.366320 0.000000

9 C 3.518044 2.233100 1.364654 0.000000

10 C 3.554094 2.292822 2.320777 1.503489 0.000000

11 C 2.479339 1.482356 2.304436 2.286053 1.349216

12 N 4.824041 5.356281 5.013613 6.262153 7.303727

13 C 6.847900 7.027325 6.259110 7.229824 8.549620

14 C 7.288920 7.224480 6.245174 7.003925 8.427680

15 C 6.270830 6.015368 4.923409 5.575700 7.027325

16 N 5.016206 4.923409 4.003613 4.912740 6.259110

17 C 5.346355 5.575700 4.912740 5.997139 7.229824

18 N 6.778984 6.270830 5.016206 5.346355 6.847900

19 N 5.011124 4.192971 2.839245 2.923420 4.426808

20 C 6.256837 5.521587 4.180518 4.236353 5.733153

21 C 7.273977 6.353869 4.988754 4.642815 6.042430

22 C 6.791543 5.706660 4.391116 3.718468 4.981816

23 C 5.347823 4.267279 2.945764 2.376310 3.768066

24 N 4.761280 3.516593 2.417022 1.316102 2.483432

25 Zn 3.389492 3.007684 2.001807 2.998569 4.274810

26 C 3.076499 4.397450 5.366933 6.575414 6.568059

27 H 4.604653 5.704620 6.049861 7.414232 7.981420

28 C 4.976958 3.758706 3.736193 2.631970 1.485296

29 H 2.837650 2.271785 3.333568 3.348581 2.186894

30 C 7.814011 8.174107 7.543666 8.596926 9.858675

31 H 8.343241 8.222891 7.182367 7.839290 9.297855

32 C 8.727588 7.836650 6.470612 6.115971 7.487786

33 H 7.497588 6.323684 5.084583 4.177480 5.223436

34 H 4.140484 5.461398 6.367659 7.612215 7.653428

35 H 3.084157 4.339745 5.412164 6.530993 6.378854

36 H 3.084157 4.339745 5.412164 6.530993 6.378854

37 H 5.567387 4.327266 4.128032 2.932766 2.135348

38 H 5.567387 4.327266 4.128032 2.932766 2.135348

39 H 5.231003 4.163092 4.455345 3.537012 2.140223

40 H 7.790891 8.251277 7.725949 8.837318 10.035176

41 H 7.790891 8.251277 7.725949 8.837318 10.035176

42 H 8.825742 9.112672 8.393102 9.367613 10.688650

43 H 9.074577 8.254792 6.899681 6.649182 8.046172

44 H 9.074577 8.254792 6.899681 6.649182 8.046172

45 H 9.362103 8.371423 7.020160 6.469335 7.732290

11 12 13 14 15

11 C 0.000000

12 N 6.836060 0.000000

13 C 8.427680 2.483432 0.000000

14 C 8.520348 3.539816 1.349216 0.000000

15 C 7.224480 3.516593 2.292822 1.482356 0.000000

16 N 6.245174 2.417022 2.320777 2.304436 1.366320

17 C 7.003925 1.316102 1.503489 2.286053 2.233100

18 N 7.288920 4.761280 3.554094 2.479339 1.321490

19 N 4.989690 5.009106 5.003677 4.414360 2.932018

20 C 6.343807 5.332278 4.659932 3.753702 2.374953

21 C 6.906041 6.798933 6.019227 4.979842 3.730244

22 C 6.000762 7.259829 6.908064 6.023360 4.638770

23 C 4.655593 6.269085 6.368815 5.730248 4.253796

24 N 3.539816 6.776998 7.303727 6.836060 5.356281

25 Zn 4.260174 3.388499 4.274810 4.260174 3.007684

26 C 5.348596 5.016288 7.487786 8.387432 7.836650

27 H 7.066905 2.865460 5.223436 6.387203 6.323684

28 C 2.571377 8.747763 9.858675 9.619655 8.174107

29 H 1.081301 7.536837 9.297855 9.477002 8.222891

30 C 9.619655 3.048288 1.485296 2.571377 3.758706

31 H 9.477002 4.565584 2.186894 1.081301 2.271785

32 C 8.387432 7.775541 6.568059 5.348596 4.397450

33 H 6.387203 8.318193 7.981420 7.066905 5.704620

34 H 6.439848 5.255369 7.732290 8.754530 8.371423

35 H 5.121629 5.615636 8.046172 8.885367 8.254792

36 H 5.121629 5.615636 8.046172 8.885367 8.254792

37 H 3.275730 9.077133 10.035176 9.710007 8.251277

38 H 3.275730 9.077133 10.035176 9.710007 8.251277

39 H 2.754389 9.398200 10.688650 10.535241 9.112672

40 H 9.710007 3.047289 2.135348 3.275730 4.327266

41 H 9.710007 3.047289 2.135348 3.275730 4.327266

42 H 10.535241 4.113086 2.140223 2.754389 4.163092

43 H 8.885367 7.766025 6.378854 5.121629 4.339745

44 H 8.885367 7.766025 6.378854 5.121629 4.339745

45 H 8.754530 8.784089 7.653428 6.439848 5.461398

16 17 18 19 20

16 N 0.000000

17 C 1.364654 0.000000

18 N 2.414426 3.518044 0.000000

19 N 2.835235 4.185912 2.439540 0.000000

20 C 2.928094 4.251136 1.365762 1.355241 0.000000

21 C 4.395548 5.711494 2.502125 2.293241 1.467670

22 C 4.972364 6.336219 3.583866 2.281210 2.272333

23 C 4.189160 5.527034 3.548271 1.366680 2.219878

24 N 5.013613 6.262153 4.824041 2.440926 3.544948

25 Zn 2.001807 2.998569 3.389492 2.010648 3.002999

26 C 6.470612 6.115971 8.727588 7.543988 8.593436

27 H 5.084583 4.177480 7.497588 7.178342 7.834592

28 C 7.543666 8.596926 7.814011 5.379941 6.578478

29 H 7.182367 7.839290 8.343241 6.066145 7.420972

30 C 3.736193 2.631970 4.976958 6.480217 6.132797

31 H 3.333568 3.348581 2.837650 5.096264 4.201165

32 C 5.366933 6.575414 3.076499 3.719138 2.616714

33 H 6.049861 7.414232 4.604653 3.316046 3.330842

34 H 7.020160 6.469335 9.362103 8.384476 9.354810

35 H 6.899681 6.649182 9.074577 7.742261 8.848679

36 H 6.899681 6.649182 9.074577 7.742261 8.848679

37 H 7.725949 8.837318 7.790891 5.407822 6.517293

38 H 7.725949 8.837318 7.790891 5.407822 6.517293

39 H 8.393102 9.367613 8.825742 6.386271 7.619506

40 H 4.128032 2.932766 5.567387 6.896183 6.654124

41 H 4.128032 2.932766 5.567387 6.896183 6.654124

42 H 4.455345 3.537012 5.231003 7.041360 6.500687

43 H 5.412164 6.530993 3.084157 4.126193 2.935907

44 H 5.412164 6.530993 3.084157 4.126193 2.935907

45 H 6.367659 7.612215 4.140484 4.427329 3.512661

21 22 23 24 25

21 C 0.000000

22 C 1.374957 0.000000

23 C 2.276728 1.445379 0.000000

24 N 3.596167 2.500113 1.369143 0.000000

25 Zn 4.254060 4.242160 3.017625 3.388499 0.000000

26 C 9.830372 9.588873 8.177809 7.775541 5.597246

27 H 9.261123 9.447878 8.222070 8.318193 5.217247

28 C 6.580108 5.336532 4.415380 3.048288 5.605871

29 H 7.981635 7.048431 5.724026 4.565584 5.228987

30 C 7.466445 8.388375 7.846535 8.747763 5.605871

31 H 5.212694 6.402817 6.335003 7.536837 5.228987

32 C 1.488680 2.589145 3.740841 5.016288 5.597246

33 H 2.205674 1.081101 2.247005 2.865460 5.217247

34 H 10.649901 10.497589 9.109065 8.784089 6.395908

35 H 10.024091 9.694864 8.271479 7.766025 5.868674

36 H 10.024091 9.694864 8.271479 7.766025 5.868674

37 H 6.378540 5.097191 4.340160 3.047289 5.861590

38 H 6.378540 5.097191 4.340160 3.047289 5.861590

39 H 7.665979 6.427444 5.482228 4.113086 6.414039

40 H 8.014034 8.872821 8.251764 9.077133 5.861590

41 H 8.014034 8.872821 8.251764 9.077133 5.861590

42 H 7.727006 8.772662 8.392681 9.398200 6.414039

43 H 2.143436 3.299108 4.321738 5.615636 5.868674

44 H 2.143436 3.299108 4.321738 5.615636 5.868674

45 H 2.142181 2.758209 4.129447 5.255369 6.395908

26 27 28 29 30

26 C 0.000000

27 H 2.990277 0.000000

28 C 7.918832 9.459454 0.000000

29 H 5.276246 7.391228 2.985124 0.000000

30 C 7.924771 5.273485 11.211741 10.422343 0.000000

31 H 9.460665 7.381986 10.422343 10.457975 2.985124

32 C 11.194493 10.399804 7.924771 9.460665 7.918832

33 H 10.399804 10.434495 5.273485 7.381986 9.459454

34 H 1.091365 2.740364 9.009833 6.351717 7.968046

35 H 1.095151 3.745268 7.662817 4.937642 8.544909

36 H 1.095151 3.745268 7.662817 4.937642 8.544909

37 H 8.530487 9.945456 1.094711 3.737941 11.417953

38 H 8.530487 9.945456 1.094711 3.737941 11.417953

39 H 7.978562 9.820398 1.090923 2.749348 11.997552

40 H 7.655429 4.923791 11.417953 10.460826 1.094711

41 H 7.655429 4.923791 11.417953 10.460826 1.094711

42 H 9.015580 6.346568 11.997552 11.375654 1.090923

43 H 11.416726 10.454423 8.544909 9.959265 7.662817

44 H 11.416726 10.454423 8.544909 9.959265 7.662817

45 H 11.970068 11.346586 7.968046 9.805895 9.009833

31 32 33 34 35

31 H 0.000000

32 C 5.276246 0.000000

33 H 7.391228 2.990277 0.000000

34 H 9.805895 11.970068 11.346586 0.000000

35 H 9.959265 11.416726 10.454423 1.771840 0.000000

36 H 9.959265 11.416726 10.454423 1.771840 1.754023

37 H 10.460826 7.655429 4.923791 9.614514 8.201418

38 H 10.460826 7.655429 4.923791 9.614514 8.386843

39 H 11.375654 9.015580 6.346568 9.064166 7.644514

40 H 3.737941 8.530487 9.945456 7.621867 8.201219

41 H 3.737941 8.530487 9.945456 7.621867 8.386648

42 H 2.749348 7.978562 9.820398 9.051848 9.629323

43 H 4.937642 1.095151 3.745268 12.147366 11.605547

44 H 4.937642 1.095151 3.745268 12.147366 11.737347

45 H 6.351717 1.091365 2.740364 12.791815 12.147366

36 37 38 39 40

36 H 0.000000

37 H 8.386843 0.000000

38 H 8.201418 1.753610 0.000000

39 H 7.644514 1.774813 1.774813 0.000000

40 H 8.386648 11.591281 11.723180 12.159207 0.000000

41 H 8.201219 11.723180 11.591281 12.159207 1.753610

42 H 9.629323 12.159207 12.159207 12.828078 1.774813

43 H 11.737347 8.201219 8.386648 9.629323 8.201418

44 H 11.605547 8.386648 8.201219 9.629323 8.386843

45 H 12.147366 7.621867 7.621867 9.051848 9.614514

41 42 43 44 45

41 H 0.000000

42 H 1.774813 0.000000

43 H 8.386843 7.644514 0.000000

44 H 8.201418 7.644514 1.754023 0.000000

45 H 9.614514 9.064166 1.771840 1.771840 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=0 Diff= 8.94D-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 2.806872 -1.107940 0.000000

2 7 0 2.010646 0.002842 0.000000

3 6 0 2.789578 1.111870 0.000000

4 6 0 4.196867 0.695225 0.000000

5 6 0 4.187353 -0.679699 0.000000

6 7 0 2.378907 2.414427 0.000000

7 6 0 1.113138 2.794116 0.000000

8 7 0 0.000000 2.001807 0.000000

9 6 0 -1.119926 2.781579 0.000000

10 6 0 -0.682385 4.219994 0.000000

11 6 0 0.666774 4.207671 0.000000

12 7 0 2.382371 -2.409613 0.000000

13 6 0 0.682385 -4.219994 0.000000

14 6 0 -0.666774 -4.207671 0.000000

15 6 0 -1.113138 -2.794116 0.000000

16 7 0 -0.000000 -2.001807 0.000000

17 6 0 1.119926 -2.781579 0.000000

18 7 0 -2.378907 -2.414427 0.000000

19 7 0 -2.010646 -0.002842 0.000000

20 6 0 -2.789578 -1.111870 0.000000

21 6 0 -4.196867 -0.695225 0.000000

22 6 0 -4.187353 0.679699 0.000000

23 6 0 -2.806872 1.107940 0.000000

24 7 0 -2.382371 2.409613 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 5.354152 1.631632 0.000000

27 1 0 5.041626 -1.342268 0.000000

28 6 0 -1.630126 5.363625 0.000000

29 1 0 1.338965 5.054650 0.000000

30 6 0 1.630126 -5.363625 0.000000

31 1 0 -1.338965 -5.054650 0.000000

32 6 0 -5.354152 -1.631632 0.000000

33 1 0 -5.041626 1.342268 0.000000

34 1 0 6.302177 1.090961 0.000000

35 1 0 5.333004 2.287193 0.877011

36 1 0 5.333004 2.287193 -0.877011

37 1 0 -2.284511 5.326393 0.876805

38 1 0 -2.284511 5.326393 -0.876805

39 1 0 -1.102648 6.318549 0.000000

40 1 0 2.284511 -5.326393 0.876805

41 1 0 2.284511 -5.326393 -0.876805

42 1 0 1.102648 -6.318549 0.000000

43 1 0 -5.333004 -2.287193 0.877011

44 1 0 -5.333004 -2.287193 -0.877011

45 1 0 -6.302177 -1.090961 0.000000

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

Rotational constants (GHZ): 0.1829252 0.1818372 0.0913943

Leave Link 202 at Tue Sep 17 14:18:11 2019, MaxMem= 2415919104 cpu: 0.1

(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 101 beta electrons

nuclear repulsion energy 2761.4129997256 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= -0.1142115676 Hartrees.

Nuclear repulsion after empirical dispersion term = 2761.2987881581 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 = 3498

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.20D-10

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 126

GePol: Fraction of low-weight points (<1% of avg) = 3.60%

GePol: Cavity surface area = 382.152 Ang\*\*2

GePol: Cavity volume = 379.368 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0107128833 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2761.2880752748 Hartrees.

Leave Link 301 at Tue Sep 17 14:18:11 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= 15325 LenP2D= 41260.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.85D-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 14:18:12 2019, MaxMem= 2415919104 cpu: 12.5

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:18:12 2019, MaxMem= 2415919104 cpu: 1.2

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= 0.000000 0.000000 -0.000000

Rot= 1.000000 -0.000000 -0.000000 -0.000308 Ang= -0.04 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 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0177 S= 1.0059

Leave Link 401 at Tue Sep 17 14:18:13 2019, MaxMem= 2415919104 cpu: 22.0

(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= 36708012.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.88D-15 for 3472.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.66D-15 for 2522 220.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.00D-15 for 3472.

Iteration 1 A^-1\*A deviation from orthogonality is 7.88D-12 for 1984 1970.

E= -1275.84265460518

DIIS: error= 1.33D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.84265460518 IErMin= 1 ErrMin= 1.33D-04

ErrMax= 1.33D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.30D-05 BMatP= 4.30D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.33D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.303 Goal= None Shift= 0.000

Gap= 0.393 Goal= None Shift= 0.000

RMSDP=1.04D-05 MaxDP=2.59D-04 OVMax= 3.50D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.04D-05 CP: 1.00D+00

E= -1275.84267149245 Delta-E= -0.000016887272 Rises=F Damp=F

DIIS: error= 9.20D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84267149245 IErMin= 2 ErrMin= 9.20D-05

ErrMax= 9.20D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.76D-06 BMatP= 4.30D-05

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

Coeff-Com: 0.113D+00 0.887D+00

Coeff: 0.113D+00 0.887D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=5.50D-06 MaxDP=2.57D-04 DE=-1.69D-05 OVMax= 3.70D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 5.20D-06 CP: 1.00D+00 1.17D+00

E= -1275.84267172692 Delta-E= -0.000000234470 Rises=F Damp=F

DIIS: error= 1.50D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1275.84267172692 IErMin= 2 ErrMin= 9.20D-05

ErrMax= 1.50D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.10D-05 BMatP= 4.76D-06

IDIUse=3 WtCom= 4.49D-01 WtEn= 5.51D-01

Coeff-Com: -0.174D-01 0.621D+00 0.396D+00

Coeff-En: 0.000D+00 0.465D+00 0.535D+00

Coeff: -0.781D-02 0.535D+00 0.472D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.33D-06 MaxDP=1.43D-04 DE=-2.34D-07 OVMax= 7.98D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.75D-06 CP: 1.00D+00 1.29D+00 7.17D-01

E= -1275.84267432135 Delta-E= -0.000002594428 Rises=F Damp=F

DIIS: error= 6.63D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84267432135 IErMin= 4 ErrMin= 6.63D-05

ErrMax= 6.63D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.09D-06 BMatP= 4.76D-06

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

Coeff-Com: -0.963D-02 0.138D+00 0.248D+00 0.623D+00

Coeff: -0.963D-02 0.138D+00 0.248D+00 0.623D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.29D-06 MaxDP=1.19D-04 DE=-2.59D-06 OVMax= 1.62D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 8.18D-07 CP: 1.00D+00 1.36D+00 1.10D+00 1.09D+00

E= -1275.84267508022 Delta-E= -0.000000758872 Rises=F Damp=F

DIIS: error= 3.43D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84267508022 IErMin= 5 ErrMin= 3.43D-05

ErrMax= 3.43D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.47D-07 BMatP= 1.09D-06

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

Coeff-Com: 0.338D-02-0.109D+00-0.394D-01 0.378D+00 0.767D+00

Coeff: 0.338D-02-0.109D+00-0.394D-01 0.378D+00 0.767D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.33D-06 MaxDP=1.07D-04 DE=-7.59D-07 OVMax= 1.75D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 4.38D-07 CP: 1.00D+00 1.46D+00 1.38D+00 1.58D+00 1.32D+00

E= -1275.84267566923 Delta-E= -0.000000589014 Rises=F Damp=F

DIIS: error= 2.54D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84267566923 IErMin= 6 ErrMin= 2.54D-05

ErrMax= 2.54D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.72D-07 BMatP= 3.47D-07

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

Coeff-Com: 0.143D-01-0.162D+00-0.387D+00-0.517D+00 0.148D+00 0.190D+01

Coeff: 0.143D-01-0.162D+00-0.387D+00-0.517D+00 0.148D+00 0.190D+01

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=5.78D-06 MaxDP=2.84D-04 DE=-5.89D-07 OVMax= 4.39D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 4.10D-07 CP: 1.00D+00 1.72D+00 2.12D+00 2.70D+00 2.82D+00

CP: 2.94D+00

E= -1275.84267647988 Delta-E= -0.000000810643 Rises=F Damp=F

DIIS: error= 9.24D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84267647988 IErMin= 7 ErrMin= 9.24D-06

ErrMax= 9.24D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.87D-08 BMatP= 1.72D-07

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

Coeff-Com: 0.435D-02-0.177D-01-0.153D+00-0.292D+00-0.107D+00 0.672D+00

Coeff-Com: 0.893D+00

Coeff: 0.435D-02-0.177D-01-0.153D+00-0.292D+00-0.107D+00 0.672D+00

Coeff: 0.893D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.88D-06 MaxDP=9.55D-05 DE=-8.11D-07 OVMax= 1.44D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 5.45D-07 CP: 1.00D+00 1.80D+00 2.35D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.33D+00

E= -1275.84267656472 Delta-E= -0.000000084840 Rises=F Damp=F

DIIS: error= 4.70D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84267656472 IErMin= 8 ErrMin= 4.70D-06

ErrMax= 4.70D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.25D-08 BMatP= 3.87D-08

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

Coeff-Com: -0.343D-02 0.733D-01 0.783D-01 0.721D-01-0.783D-01-0.474D+00

Coeff-Com: 0.627D+00 0.706D+00

Coeff: -0.343D-02 0.733D-01 0.783D-01 0.721D-01-0.783D-01-0.474D+00

Coeff: 0.627D+00 0.706D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.65D-07 MaxDP=2.04D-05 DE=-8.48D-08 OVMax= 2.44D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.74D-07 CP: 1.00D+00 1.80D+00 2.39D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.65D+00 1.40D+00

E= -1275.84267658001 Delta-E= -0.000000015295 Rises=F Damp=F

DIIS: error= 1.68D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84267658001 IErMin= 9 ErrMin= 1.68D-06

ErrMax= 1.68D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.89D-09 BMatP= 2.25D-08

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

Coeff-Com: -0.191D-02 0.273D-01 0.510D-01 0.786D-01 0.182D-01-0.313D+00

Coeff-Com: 0.320D-01 0.267D+00 0.841D+00

Coeff: -0.191D-02 0.273D-01 0.510D-01 0.786D-01 0.182D-01-0.313D+00

Coeff: 0.320D-01 0.267D+00 0.841D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.09D-07 MaxDP=1.17D-05 DE=-1.53D-08 OVMax= 1.48D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 6.56D-08 CP: 1.00D+00 1.81D+00 2.41D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.80D+00 1.63D+00 1.25D+00

E= -1275.84267658393 Delta-E= -0.000000003914 Rises=F Damp=F

DIIS: error= 1.21D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84267658393 IErMin=10 ErrMin= 1.21D-06

ErrMax= 1.21D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.18D-09 BMatP= 2.89D-09

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

Coeff-Com: 0.426D-04-0.866D-02 0.633D-03 0.216D-01 0.406D-01-0.331D-01

Coeff-Com: -0.183D+00-0.468D-01 0.445D+00 0.764D+00

Coeff: 0.426D-04-0.866D-02 0.633D-03 0.216D-01 0.406D-01-0.331D-01

Coeff: -0.183D+00-0.468D-01 0.445D+00 0.764D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.64D-07 MaxDP=9.19D-06 DE=-3.91D-09 OVMax= 1.22D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 4.19D-08 CP: 1.00D+00 1.82D+00 2.43D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.89D+00 1.78D+00 1.57D+00 1.40D+00

E= -1275.84267658562 Delta-E= -0.000000001698 Rises=F Damp=F

DIIS: error= 7.07D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84267658562 IErMin=11 ErrMin= 7.07D-07

ErrMax= 7.07D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.16D-10 BMatP= 1.18D-09

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

Coeff-Com: 0.533D-03-0.117D-01-0.139D-01-0.524D-02 0.163D-01 0.652D-01

Coeff-Com: -0.114D+00-0.867D-01-0.534D-01 0.387D+00 0.815D+00

Coeff: 0.533D-03-0.117D-01-0.139D-01-0.524D-02 0.163D-01 0.652D-01

Coeff: -0.114D+00-0.867D-01-0.534D-01 0.387D+00 0.815D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=8.39D-08 MaxDP=4.23D-06 DE=-1.70D-09 OVMax= 5.84D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.81D-08 CP: 1.00D+00 1.82D+00 2.44D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.93D+00 1.86D+00 1.74D+00 1.90D+00

CP: 1.24D+00

E= -1275.84267658611 Delta-E= -0.000000000488 Rises=F Damp=F

DIIS: error= 3.50D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84267658611 IErMin=12 ErrMin= 3.50D-07

ErrMax= 3.50D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.61D-10 BMatP= 4.16D-10

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

Coeff-Com: 0.328D-03-0.431D-02-0.103D-01-0.120D-01-0.701D-02 0.541D-01

Coeff-Com: -0.275D-02-0.274D-01-0.211D+00-0.400D-01 0.515D+00 0.746D+00

Coeff: 0.328D-03-0.431D-02-0.103D-01-0.120D-01-0.701D-02 0.541D-01

Coeff: -0.275D-02-0.274D-01-0.211D+00-0.400D-01 0.515D+00 0.746D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=7.99D-08 MaxDP=4.15D-06 DE=-4.88D-10 OVMax= 6.04D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.45D-08 CP: 1.00D+00 1.82D+00 2.45D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.96D+00 1.92D+00 1.90D+00 2.20D+00

CP: 1.68D+00 1.04D+00

E= -1275.84267658632 Delta-E= -0.000000000211 Rises=F Damp=F

DIIS: error= 1.16D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84267658632 IErMin=13 ErrMin= 1.16D-07

ErrMax= 1.16D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.80D-11 BMatP= 1.61D-10

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

Coeff-Com: 0.204D-04 0.117D-02-0.117D-02-0.394D-02-0.789D-02 0.670D-02

Coeff-Com: 0.276D-01 0.120D-01-0.857D-01-0.114D+00 0.351D-01 0.340D+00

Coeff-Com: 0.790D+00

Coeff: 0.204D-04 0.117D-02-0.117D-02-0.394D-02-0.789D-02 0.670D-02

Coeff: 0.276D-01 0.120D-01-0.857D-01-0.114D+00 0.351D-01 0.340D+00

Coeff: 0.790D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.25D-08 MaxDP=1.66D-06 DE=-2.11D-10 OVMax= 2.46D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 5.16D-09 CP: 1.00D+00 1.82D+00 2.45D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.97D+00 1.95D+00 1.95D+00 2.31D+00

CP: 1.84D+00 1.20D+00 1.32D+00

E= -1275.84267658633 Delta-E= -0.000000000009 Rises=F Damp=F

DIIS: error= 6.11D-08 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84267658633 IErMin=14 ErrMin= 6.11D-08

ErrMax= 6.11D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.29D-12 BMatP= 1.80D-11

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

Coeff-Com: -0.267D-04 0.123D-02 0.717D-03-0.622D-03-0.349D-02-0.304D-02

Coeff-Com: 0.165D-01 0.977D-02-0.242D-01-0.621D-01-0.460D-01 0.114D+00

Coeff-Com: 0.458D+00 0.540D+00

Coeff: -0.267D-04 0.123D-02 0.717D-03-0.622D-03-0.349D-02-0.304D-02

Coeff: 0.165D-01 0.977D-02-0.242D-01-0.621D-01-0.460D-01 0.114D+00

Coeff: 0.458D+00 0.540D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.67D-09 MaxDP=1.66D-07 DE=-9.09D-12 OVMax= 7.64D-07

Error on total polarization charges = 0.06464

SCF Done: E(UB3LYP) = -1275.84267659 A.U. after 14 cycles

NFock= 14 Conv=0.27D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0178 S= 1.0059

<L.S>= 0.000000000000E+00

KE= 1.320801934832D+03 PE=-8.574527179884D+03 EE= 3.216594493190D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.72

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0178, after 2.0002

Leave Link 502 at Tue Sep 17 14:19:26 2019, MaxMem= 2415919104 cpu: 1272.7

(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= 41260.

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 = 246

Leave Link 701 at Tue Sep 17 14:19:30 2019, MaxMem= 2415919104 cpu: 74.4

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 14:19:30 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 14:19:40 2019, MaxMem= 2415919104 cpu: 176.9

(Enter /home/blab/g09/l716.exe)

Dipole = 1.90070182D-13 1.40776280D-13 4.44089210D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000049472 0.000384318 0.000000000

2 7 -0.000266966 0.000147273 -0.000000000

3 6 0.000473126 -0.000110113 -0.000000000

4 6 -0.000146243 -0.000025852 -0.000000000

5 6 -0.000024068 -0.000259477 -0.000000000

6 7 -0.000402121 -0.000048394 -0.000000000

7 6 0.000283809 -0.000072039 0.000000000

8 7 0.000212867 0.000208519 -0.000000000

9 6 -0.000143781 -0.000466605 -0.000000000

10 6 0.000041865 0.000289117 -0.000000000

11 6 -0.000265744 -0.000134017 -0.000000000

12 7 0.000048876 -0.000468747 -0.000000000

13 6 -0.000041865 -0.000289117 -0.000000000

14 6 0.000265744 0.000134017 0.000000000

15 6 -0.000283809 0.000072039 -0.000000000

16 7 -0.000212867 -0.000208519 0.000000000

17 6 0.000143781 0.000466605 -0.000000000

18 7 0.000402121 0.000048394 -0.000000000

19 7 0.000266966 -0.000147273 -0.000000000

20 6 -0.000473126 0.000110113 -0.000000000

21 6 0.000146243 0.000025852 -0.000000000

22 6 0.000024068 0.000259477 -0.000000000

23 6 -0.000049472 -0.000384318 0.000000000

24 7 -0.000048876 0.000468747 0.000000000

25 30 0.000000000 -0.000000000 0.000000000

26 6 -0.000011450 -0.000010410 -0.000000000

27 1 -0.000030322 -0.000021695 0.000000000

28 6 0.000028383 0.000007541 -0.000000000

29 1 -0.000022037 0.000037041 0.000000000

30 6 -0.000028383 -0.000007541 0.000000000

31 1 0.000022037 -0.000037041 0.000000000

32 6 0.000011450 0.000010410 0.000000000

33 1 0.000030322 0.000021695 0.000000000

34 1 -0.000000991 0.000002230 -0.000000000

35 1 -0.000005160 0.000011934 0.000011585

36 1 -0.000005160 0.000011934 -0.000011585

37 1 0.000011522 0.000005897 0.000015547

38 1 0.000011522 0.000005897 -0.000015547

39 1 0.000029464 0.000002026 -0.000000000

40 1 -0.000011522 -0.000005897 0.000015547

41 1 -0.000011522 -0.000005897 -0.000015547

42 1 -0.000029464 -0.000002026 -0.000000000

43 1 0.000005160 -0.000011934 0.000011585

44 1 0.000005160 -0.000011934 -0.000011585

45 1 0.000000991 -0.000002230 0.000000000

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

Cartesian Forces: Max 0.000473126 RMS 0.000151472

Leave Link 716 at Tue Sep 17 14:19:40 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 0.000272890 RMS 0.000061177

Search for a local minimum.

Step number 17 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 12 13 14 15

16 17

DE= -2.78D-07 DEPred=-2.96D-06 R= 9.38D-02

Trust test= 9.38D-02 RLast= 1.12D-02 DXMaxT set to 7.92D-02

ITU= -1 1 1 -1 1 1 1 -1 0 1 -1 1 1 1 1 0 0

Eigenvalues --- 0.00137 0.00878 0.00878 0.00878 0.00878

Eigenvalues --- 0.01337 0.01338 0.01346 0.01347 0.01604

Eigenvalues --- 0.01623 0.01631 0.01640 0.01774 0.01793

Eigenvalues --- 0.01809 0.01823 0.01890 0.01909 0.01939

Eigenvalues --- 0.01950 0.01997 0.02000 0.02045 0.02047

Eigenvalues --- 0.02070 0.02087 0.02103 0.02110 0.02115

Eigenvalues --- 0.02205 0.02312 0.02316 0.02351 0.02372

Eigenvalues --- 0.07195 0.07195 0.07200 0.07200 0.07255

Eigenvalues --- 0.07312 0.07391 0.07435 0.09359 0.13678

Eigenvalues --- 0.14497 0.14500 0.14672 0.15746 0.15986

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16025 0.16231 0.16406 0.17650 0.18803

Eigenvalues --- 0.21496 0.22061 0.22094 0.23677 0.23841

Eigenvalues --- 0.23853 0.23893 0.24867 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25001

Eigenvalues --- 0.25969 0.27962 0.29709 0.32161 0.33169

Eigenvalues --- 0.33189 0.33198 0.33282 0.33282 0.33630

Eigenvalues --- 0.33697 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33724 0.33879 0.34256 0.34437

Eigenvalues --- 0.34437 0.34440 0.34669 0.35089 0.35554

Eigenvalues --- 0.35564 0.35671 0.35682 0.35682 0.35867

Eigenvalues --- 0.38664 0.39733 0.41184 0.41637 0.41819

Eigenvalues --- 0.46713 0.48682 0.48966 0.48982 0.50806

Eigenvalues --- 0.51358 0.51361 0.52774 0.53676 0.54018

Eigenvalues --- 0.54027 0.56320 0.56330 0.57164

Cosine: 0.224 < 0.500

Cut down GDIIS temporarily because of the cosine check. E 7

DIIS coeff's: 1.34242 0.72624 -0.82470 -0.24395

Cosine: 0.924 > 0.500

Length: 0.348

GDIIS step was calculated using 4 of the last 17 vectors.

Maximum step size ( 0.079) exceeded in Quadratic search.

-- Step size scaled by 0.935

Iteration 1 RMS(Cart)= 0.01234149 RMS(Int)= 0.00003887

Iteration 2 RMS(Cart)= 0.00006487 RMS(Int)= 0.00000377

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000377

ITry= 1 IFail=0 DXMaxC= 5.83D-02 DCOld= 1.00D+10 DXMaxT= 7.92D-02 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 6.79D-10 for atom 36.

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

(Linear) (Quad) (Total)

R1 2.58265 -0.00007 -0.00167 0.00237 0.00069 2.58334

R2 2.73137 0.00021 -0.00005 -0.00510 -0.00514 2.72623

R3 2.58730 -0.00022 0.00086 -0.02576 -0.02490 2.56241

R4 2.56103 0.00018 0.00071 -0.00871 -0.00800 2.55303

R5 3.79957 0.00003 0.00281 0.00164 0.00445 3.80402

R6 2.77349 0.00015 -0.00081 0.00372 0.00291 2.77640

R7 2.58092 -0.00022 -0.00032 -0.00859 -0.00890 2.57201

R8 2.59829 -0.00007 0.00072 0.00015 0.00087 2.59916

R9 2.81320 -0.00002 0.00079 -0.00464 -0.00385 2.80935

R10 2.04298 0.00004 0.00013 0.00092 0.00104 2.04403

R11 2.49725 0.00020 -0.00090 0.00488 0.00398 2.50123

R12 2.58197 0.00009 0.00080 -0.00619 -0.00539 2.57658

R13 2.80125 -0.00014 -0.00046 -0.00295 -0.00342 2.79782

R14 2.57882 -0.00012 -0.00163 -0.00023 -0.00185 2.57697

R15 3.78287 0.00006 0.00336 0.00087 0.00423 3.78709

R16 2.84118 -0.00010 0.00063 -0.01081 -0.01017 2.83101

R17 2.48707 0.00027 0.00037 0.00084 0.00121 2.48828

R18 2.54965 0.00023 0.00068 0.00965 0.01033 2.55998

R19 2.80680 0.00008 -0.00010 0.00171 0.00161 2.80841

R20 2.04336 -0.00004 0.00039 -0.00187 -0.00149 2.04188

R21 2.48707 0.00027 0.00037 0.00084 0.00121 2.48828

R22 2.54965 0.00023 0.00068 0.00965 0.01033 2.55998

R23 2.84118 -0.00010 0.00063 -0.01081 -0.01017 2.83101

R24 2.80680 0.00008 -0.00010 0.00171 0.00161 2.80841

R25 2.80125 -0.00014 -0.00046 -0.00295 -0.00342 2.79782

R26 2.04336 -0.00004 0.00039 -0.00187 -0.00149 2.04188

R27 2.58197 0.00009 0.00080 -0.00619 -0.00539 2.57658

R28 2.49725 0.00020 -0.00090 0.00488 0.00398 2.50123

R29 2.57882 -0.00012 -0.00163 -0.00023 -0.00185 2.57697

R30 3.78287 0.00006 0.00336 0.00087 0.00423 3.78709

R31 2.58092 -0.00022 -0.00032 -0.00859 -0.00890 2.57201

R32 2.56103 0.00018 0.00071 -0.00871 -0.00800 2.55303

R33 2.58265 -0.00007 -0.00167 0.00237 0.00069 2.58334

R34 3.79957 0.00003 0.00281 0.00164 0.00445 3.80402

R35 2.77349 0.00015 -0.00081 0.00372 0.00291 2.77640

R36 2.59829 -0.00007 0.00072 0.00015 0.00087 2.59916

R37 2.81320 -0.00002 0.00079 -0.00464 -0.00385 2.80935

R38 2.73137 0.00021 -0.00005 -0.00510 -0.00514 2.72623

R39 2.04298 0.00004 0.00013 0.00092 0.00104 2.04403

R40 2.58730 -0.00022 0.00086 -0.02576 -0.02490 2.56241

R41 2.06238 -0.00000 0.00027 0.00073 0.00099 2.06337

R42 2.06954 0.00000 0.00050 0.00083 0.00133 2.07086

R43 2.06954 0.00000 0.00050 0.00083 0.00133 2.07086

R44 2.06870 0.00002 0.00042 0.00034 0.00076 2.06947

R45 2.06870 0.00002 0.00042 0.00034 0.00076 2.06947

R46 2.06155 0.00002 0.00020 0.00115 0.00135 2.06290

R47 2.06870 0.00002 0.00042 0.00034 0.00076 2.06947

R48 2.06870 0.00002 0.00042 0.00034 0.00076 2.06947

R49 2.06155 0.00002 0.00020 0.00115 0.00135 2.06290

R50 2.06954 0.00000 0.00050 0.00083 0.00133 2.07086

R51 2.06954 0.00000 0.00050 0.00083 0.00133 2.07086

R52 2.06238 -0.00000 0.00027 0.00073 0.00099 2.06337

A1 1.89192 0.00005 -0.00026 0.00199 0.00172 1.89364

A2 2.20443 0.00004 -0.00059 -0.00077 -0.00137 2.20306

A3 2.18684 -0.00009 0.00086 -0.00121 -0.00035 2.18649

A4 1.90736 -0.00002 0.00061 0.00522 0.00584 1.91321

A5 2.19131 0.00006 0.00011 0.00463 0.00474 2.19604

A6 2.18452 -0.00004 -0.00071 -0.00986 -0.01058 2.17394

A7 1.89526 -0.00004 -0.00021 -0.00819 -0.00840 1.88686

A8 2.22387 -0.00000 -0.00117 0.00559 0.00442 2.22829

A9 2.16405 0.00004 0.00138 0.00260 0.00398 2.16803

A10 1.85172 0.00005 -0.00036 0.00790 0.00754 1.85926

A11 2.17346 -0.00000 -0.00003 -0.01592 -0.01595 2.15752

A12 2.25801 -0.00004 0.00039 0.00801 0.00840 2.26641

A13 1.87851 -0.00004 0.00023 -0.00693 -0.00671 1.87181

A14 2.18111 0.00002 -0.00035 -0.00346 -0.00381 2.17731

A15 2.22356 0.00002 0.00012 0.01039 0.01051 2.23407

A16 2.16764 0.00007 0.00325 0.00545 0.00871 2.17635

A17 2.23158 -0.00003 -0.00093 -0.00252 -0.00344 2.22814

A18 2.16809 0.00009 0.00107 0.00841 0.00949 2.17757

A19 1.88352 -0.00006 -0.00014 -0.00589 -0.00605 1.87747

A20 1.91479 0.00005 0.00059 0.00287 0.00346 1.91825

A21 2.18938 -0.00007 -0.00104 -0.00625 -0.00730 2.18208

A22 2.17902 0.00002 0.00046 0.00338 0.00384 2.18285

A23 1.88373 0.00005 -0.00024 0.00535 0.00512 1.88885

A24 2.24684 0.00000 -0.00116 -0.00335 -0.00451 2.24234

A25 2.15262 -0.00005 0.00140 -0.00201 -0.00062 2.15200

A26 1.85695 -0.00008 0.00012 -0.00882 -0.00870 1.84825

A27 2.15430 0.00004 -0.00002 -0.00228 -0.00230 2.15200

A28 2.27193 0.00004 -0.00010 0.01110 0.01100 2.28294

A29 1.88579 0.00004 -0.00032 0.00650 0.00616 1.89196

A30 2.16488 -0.00002 0.00036 -0.00338 -0.00302 2.16186

A31 2.23251 -0.00002 -0.00003 -0.00312 -0.00315 2.22936

A32 2.17257 -0.00006 0.00179 0.00370 0.00548 2.17806

A33 1.85695 -0.00008 0.00012 -0.00882 -0.00870 1.84825

A34 2.27193 0.00004 -0.00010 0.01110 0.01100 2.28294

A35 2.15430 0.00004 -0.00002 -0.00228 -0.00230 2.15200

A36 1.88579 0.00004 -0.00032 0.00650 0.00616 1.89196

A37 2.23251 -0.00002 -0.00003 -0.00312 -0.00315 2.22936

A38 2.16488 -0.00002 0.00036 -0.00338 -0.00302 2.16186

A39 1.88352 -0.00006 -0.00014 -0.00589 -0.00605 1.87747

A40 2.16809 0.00009 0.00107 0.00841 0.00949 2.17757

A41 2.23158 -0.00003 -0.00093 -0.00252 -0.00344 2.22814

A42 1.91479 0.00005 0.00059 0.00287 0.00346 1.91825

A43 2.18938 -0.00007 -0.00104 -0.00625 -0.00730 2.18208

A44 2.17902 0.00002 0.00046 0.00338 0.00384 2.18285

A45 2.15262 -0.00005 0.00140 -0.00201 -0.00062 2.15200

A46 2.24684 0.00000 -0.00116 -0.00335 -0.00451 2.24234

A47 1.88373 0.00005 -0.00024 0.00535 0.00512 1.88885

A48 2.16764 0.00007 0.00325 0.00545 0.00871 2.17635

A49 1.90736 -0.00002 0.00061 0.00522 0.00584 1.91321

A50 2.18452 -0.00004 -0.00071 -0.00986 -0.01058 2.17394

A51 2.19131 0.00006 0.00011 0.00463 0.00474 2.19604

A52 2.22387 -0.00000 -0.00117 0.00559 0.00442 2.22829

A53 2.16405 0.00004 0.00138 0.00260 0.00398 2.16803

A54 1.89526 -0.00004 -0.00021 -0.00819 -0.00840 1.88686

A55 1.85172 0.00005 -0.00036 0.00790 0.00754 1.85926

A56 2.17346 -0.00000 -0.00003 -0.01592 -0.01595 2.15752

A57 2.25801 -0.00004 0.00039 0.00801 0.00840 2.26641

A58 1.87851 -0.00004 0.00023 -0.00693 -0.00671 1.87181

A59 2.22356 0.00002 0.00012 0.01039 0.01051 2.23407

A60 2.18111 0.00002 -0.00035 -0.00346 -0.00381 2.17731

A61 1.89192 0.00005 -0.00026 0.00199 0.00172 1.89364

A62 2.20443 0.00004 -0.00059 -0.00077 -0.00137 2.20306

A63 2.18684 -0.00009 0.00086 -0.00121 -0.00035 2.18649

A64 2.17257 -0.00006 0.00179 0.00370 0.00548 2.17806

A65 1.56938 0.00007 0.00060 0.00759 0.00819 1.57757

A66 1.57221 -0.00007 -0.00060 -0.00759 -0.00819 1.56402

A67 1.57221 -0.00007 -0.00060 -0.00759 -0.00819 1.56402

A68 1.56938 0.00007 0.00060 0.00759 0.00819 1.57757

A69 1.94300 0.00000 -0.00046 0.00065 0.00018 1.94318

A70 1.94069 -0.00002 0.00011 -0.00553 -0.00542 1.93527

A71 1.94069 -0.00002 0.00011 -0.00553 -0.00542 1.93527

A72 1.88949 0.00001 -0.00028 0.00018 -0.00011 1.88938

A73 1.88949 0.00001 -0.00028 0.00018 -0.00011 1.88938

A74 1.85730 0.00002 0.00083 0.01072 0.01155 1.86885

A75 1.93397 0.00000 -0.00027 -0.00507 -0.00534 1.92862

A76 1.93397 0.00000 -0.00027 -0.00507 -0.00534 1.92862

A77 1.94492 0.00003 -0.00061 0.00108 0.00046 1.94538

A78 1.85775 -0.00000 0.00112 0.01119 0.01231 1.87006

A79 1.89526 -0.00002 0.00006 -0.00079 -0.00073 1.89453

A80 1.89526 -0.00002 0.00006 -0.00079 -0.00073 1.89453

A81 1.93397 0.00000 -0.00027 -0.00507 -0.00534 1.92862

A82 1.93397 0.00000 -0.00027 -0.00507 -0.00534 1.92862

A83 1.94492 0.00003 -0.00061 0.00108 0.00046 1.94538

A84 1.85775 -0.00000 0.00112 0.01119 0.01231 1.87006

A85 1.89526 -0.00002 0.00006 -0.00079 -0.00073 1.89453

A86 1.89526 -0.00002 0.00006 -0.00079 -0.00073 1.89453

A87 1.94069 -0.00002 0.00011 -0.00553 -0.00542 1.93527

A88 1.94069 -0.00002 0.00011 -0.00553 -0.00542 1.93527

A89 1.94300 0.00000 -0.00046 0.00065 0.00018 1.94318

A90 1.85730 0.00002 0.00083 0.01072 0.01155 1.86885

A91 1.88949 0.00001 -0.00028 0.00018 -0.00011 1.88938

A92 1.88949 0.00001 -0.00028 0.00018 -0.00011 1.88938

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

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D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D9 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

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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

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D26 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

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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 1.03313 0.00000 0.00059 0.00313 0.00372 1.03685

D31 -1.03313 -0.00000 -0.00059 -0.00313 -0.00372 -1.03685

D32 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.10846 0.00000 0.00059 0.00313 0.00372 -2.10475

D34 2.10846 -0.00000 -0.00059 -0.00313 -0.00372 2.10475

D35 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

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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

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D62 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D63 1.02909 0.00000 0.00052 0.00375 0.00427 1.03337

D64 -1.02909 -0.00000 -0.00052 -0.00375 -0.00427 -1.03337

D65 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D66 -2.11250 0.00000 0.00052 0.00375 0.00427 -2.10823

D67 2.11250 -0.00000 -0.00052 -0.00375 -0.00427 2.10823

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 -2.11250 0.00000 0.00052 0.00375 0.00427 -2.10823

D80 2.11250 -0.00000 -0.00052 -0.00375 -0.00427 2.10823

D81 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D82 1.02909 0.00000 0.00052 0.00375 0.00427 1.03337

D83 -1.02909 -0.00000 -0.00052 -0.00375 -0.00427 -1.03337

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D89 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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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 1.03313 0.00000 0.00059 0.00313 0.00372 1.03685

D126 -1.03313 -0.00000 -0.00059 -0.00313 -0.00372 -1.03685

D127 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D128 -2.10846 0.00000 0.00059 0.00313 0.00372 -2.10475

D129 2.10846 -0.00000 -0.00059 -0.00313 -0.00372 2.10475

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 0.000273 0.000450 YES

RMS Force 0.000061 0.000300 YES

Maximum Displacement 0.058252 0.001800 NO

RMS Displacement 0.012369 0.001200 NO

Predicted change in Energy=-2.990480D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:19:40 2019, MaxMem= 2415919104 cpu: 1.3

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.086860 -2.187993 0.000000

2 7 0 -0.758620 -1.864583 0.000000

3 6 0 -0.016823 -2.993722 0.000000

4 6 0 -0.933186 -4.142137 0.000000

5 6 0 -2.207910 -3.625562 0.000000

6 7 0 1.340273 -3.097396 0.000000

7 6 0 2.174391 -2.069703 0.000000

8 7 0 1.861356 -0.742657 0.000000

9 6 0 3.002688 0.003649 0.000000

10 6 0 4.173543 -0.930921 0.000000

11 6 0 3.650771 -2.180671 0.000000

12 7 0 -3.124228 -1.314771 0.000000

13 6 0 -4.173543 0.930921 0.000000

14 6 0 -3.650771 2.180671 0.000000

15 6 0 -2.174391 2.069703 0.000000

16 7 0 -1.861356 0.742657 0.000000

17 6 0 -3.002688 -0.003649 0.000000

18 7 0 -1.340273 3.097396 0.000000

19 7 0 0.758620 1.864583 0.000000

20 6 0 0.016823 2.993722 0.000000

21 6 0 0.933186 4.142137 0.000000

22 6 0 2.207910 3.625562 0.000000

23 6 0 2.086860 2.187993 0.000000

24 7 0 3.124228 1.314771 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.478831 -5.557646 0.000000

27 1 0 -3.145241 -4.165362 0.000000

28 6 0 5.586126 -0.469134 0.000000

29 1 0 4.183947 -3.120479 0.000000

30 6 0 -5.586126 0.469134 0.000000

31 1 0 -4.183947 3.120479 0.000000

32 6 0 0.478831 5.557646 0.000000

33 1 0 3.145241 4.165362 0.000000

34 1 0 -1.325807 -6.246742 0.000000

35 1 0 0.136707 -5.770328 0.881350

36 1 0 0.136707 -5.770328 -0.881350

37 1 0 5.787526 0.149167 0.881146

38 1 0 5.787526 0.149167 -0.881146

39 1 0 6.281450 -1.310679 0.000000

40 1 0 -5.787526 -0.149167 0.881146

41 1 0 -5.787526 -0.149167 -0.881146

42 1 0 -6.281450 1.310679 0.000000

43 1 0 -0.136707 5.770328 0.881350

44 1 0 -0.136707 5.770328 -0.881350

45 1 0 1.325807 6.246742 0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.367046 0.000000

3 C 2.221318 1.351006 0.000000

4 C 2.269282 2.284234 1.469209 0.000000

5 C 1.442656 2.280677 2.280369 1.375417 0.000000

6 N 3.545737 2.434170 1.361050 2.502018 3.587277

7 C 4.262893 2.940175 2.378073 3.735239 4.650297

8 N 4.204451 2.850087 2.931698 4.400673 4.986990

9 C 5.541371 4.199730 4.254607 5.716523 6.349921

10 C 6.385365 5.019757 4.670580 6.032461 6.927051

11 C 5.737636 4.420707 3.756634 4.985981 6.034224

12 N 1.355968 2.428661 3.531974 3.576963 2.485839

13 C 3.752582 4.413223 5.716743 6.019621 4.962384

14 C 4.640156 4.972788 6.322968 6.882091 5.982825

15 C 4.258596 4.181269 5.503942 6.334631 5.695364

16 N 2.939313 2.830853 4.166873 4.972194 4.381945

17 C 2.368565 2.915290 4.225627 4.627086 3.708090

18 N 5.337859 4.995954 6.233237 7.250969 6.778714

19 N 4.951781 4.026002 4.919800 6.240423 6.240352

20 C 5.592464 4.919800 5.987539 7.198819 6.983148

21 C 7.013645 6.240423 7.198819 8.491909 8.378760

22 C 7.227896 6.240352 6.983148 8.378760 8.489892

23 C 6.047247 4.951781 5.592464 7.013645 7.227896

24 N 6.278917 5.018446 5.331914 6.800032 7.269015

25 Zn 3.023624 2.013001 2.993769 4.245955 4.244946

26 C 3.733673 3.703646 2.605217 1.486642 2.592810

27 H 2.242801 3.315048 3.340619 2.212177 1.081653

28 C 7.863154 6.496390 6.145452 7.482805 8.408926

29 H 6.339759 5.099632 4.202682 5.218125 6.411781

30 C 4.393766 5.362000 6.558086 6.550852 5.308378

31 H 5.707683 6.048446 7.399214 7.956948 7.029494

32 C 8.159516 7.524677 8.565720 9.802018 9.568170

33 H 8.230431 7.183339 7.826310 9.254625 9.452762

34 H 4.129484 4.418712 3.506505 2.140914 2.765626

35 H 4.307453 4.102833 2.917172 2.138330 3.297579

36 H 4.307453 4.102833 2.917172 2.138330 3.297579

37 H 8.261034 6.905333 6.659177 8.022447 8.885493

38 H 8.261034 6.905333 6.659177 8.022447 8.885493

39 H 8.414172 7.061827 6.519270 7.750362 8.799313

40 H 4.316035 5.385997 6.493760 6.347034 5.067089

41 H 4.316035 5.385997 6.493760 6.347034 5.067089

42 H 5.462169 6.370552 7.600882 7.637874 6.400016

43 H 8.241041 7.710734 8.809071 9.983392 9.661750

44 H 8.241041 7.710734 8.809071 9.983392 9.661750

45 H 9.098959 8.374868 9.337495 10.631643 10.485682

6 7 8 9 10

6 N 0.000000

7 C 1.323596 0.000000

8 N 2.411706 1.363467 0.000000

9 C 3.518537 2.232681 1.363675 0.000000

10 C 3.566656 2.300747 2.319839 1.498106 0.000000

11 C 2.485717 1.480545 2.295624 2.278435 1.354683

12 N 4.807236 5.352129 5.018303 6.267163 7.307859

13 C 6.828580 7.021397 6.262657 7.235892 8.552211

14 C 7.264194 7.210978 6.239343 7.000568 8.420327

15 C 6.249142 6.003881 4.919007 5.574112 7.021397

16 N 4.999644 4.919007 4.008085 4.919864 6.262657

17 C 5.332221 5.574112 4.919864 6.005381 7.235892

18 N 6.749873 6.249142 4.999644 5.332221 6.828580

19 N 4.995954 4.181269 2.830853 2.915290 4.413223

20 C 6.233237 5.503942 4.166873 4.225627 5.716743

21 C 7.250969 6.334631 4.972194 4.627086 6.019621

22 C 6.778714 5.695364 4.381945 3.708090 4.962384

23 C 5.337859 4.258596 2.939313 2.368565 3.752582

24 N 4.759172 3.515232 2.414095 1.316743 2.478749

25 Zn 3.374936 3.001941 2.004043 3.002690 4.276105

26 C 3.059732 4.382388 5.353559 6.561171 6.561339

27 H 4.610898 5.717540 6.064727 7.428167 8.001637

28 C 4.993499 3.768522 3.734799 2.626342 1.486148

29 H 2.843768 2.267696 3.323923 3.339991 2.189582

30 C 7.790708 8.165250 7.545424 8.601418 9.859579

31 H 8.317390 8.207707 7.174225 7.833412 9.287706

32 C 8.697806 7.813538 6.450209 6.100552 7.466753

33 H 7.483687 6.310197 5.073165 4.164154 5.198991

34 H 4.126301 5.449682 6.360264 7.602845 7.648582

35 H 3.061031 4.315502 5.387826 6.506108 6.363387

36 H 3.061031 4.315502 5.387826 6.506108 6.363387

37 H 5.576258 4.330652 4.121477 2.924537 2.132592

38 H 5.576258 4.330652 4.121477 2.924537 2.132592

39 H 5.254293 4.176607 4.456442 3.532384 2.141842

40 H 7.763632 8.237536 7.722308 8.835589 10.030476

41 H 7.763632 8.237536 7.722308 8.835589 10.030476

42 H 8.804645 9.106494 8.397707 9.375689 10.692598

43 H 9.032983 8.220952 6.869353 6.624739 8.016344

44 H 9.032983 8.220952 6.869353 6.624739 8.016344

45 H 9.344149 8.359626 7.009886 6.464375 7.721945

11 12 13 14 15

11 C 0.000000

12 N 6.830110 0.000000

13 C 8.420327 2.478749 0.000000

14 C 8.504930 3.534878 1.354683 0.000000

15 C 7.210978 3.515232 2.300747 1.480545 0.000000

16 N 6.239343 2.414095 2.319839 2.295624 1.363467

17 C 7.000568 1.316743 1.498106 2.278435 2.232681

18 N 7.264194 4.759172 3.566656 2.485717 1.323596

19 N 4.972788 5.018446 5.019757 4.420707 2.940175

20 C 6.322968 5.331914 4.670580 3.756634 2.378073

21 C 6.882091 6.800032 6.032461 4.985981 3.735239

22 C 5.982825 7.269015 6.927051 6.034224 4.650297

23 C 4.640156 6.278917 6.385365 5.737636 4.262893

24 N 3.534878 6.779210 7.307859 6.830110 5.352129

25 Zn 4.252465 3.389605 4.276105 4.252465 3.001941

26 C 5.334564 5.000012 7.466753 8.363179 7.813538

27 H 7.079885 2.850668 5.198991 6.366137 6.310197

28 C 2.583594 8.751306 9.859579 9.609461 8.165250

29 H 1.080515 7.527948 9.287706 9.459651 8.207707

30 C 9.609461 3.040272 1.486148 2.583594 3.768522

31 H 9.459651 4.560092 2.189582 1.080515 2.267696

32 C 8.363179 7.759648 6.561339 5.334564 4.382388

33 H 6.366137 8.326949 8.001637 7.079885 5.717540

34 H 6.426450 5.249634 7.721945 8.742239 8.359626

35 H 5.100104 5.591285 8.016344 8.850998 8.220952

36 H 5.100104 5.591285 8.016344 8.850998 8.220952

37 H 3.281811 9.074077 10.030476 9.694580 8.237536

38 H 3.281811 9.074077 10.030476 9.694580 8.237536

39 H 2.770804 9.405679 10.692598 10.527989 9.106494

40 H 9.694580 3.037796 2.132592 3.281811 4.330652

41 H 9.694580 3.037796 2.132592 3.281811 4.330652

42 H 10.527989 4.106219 2.141842 2.770804 4.176607

43 H 8.850998 7.739554 6.363387 5.100104 4.315502

44 H 8.850998 7.739554 6.363387 5.100104 4.315502

45 H 8.742239 8.773784 7.648582 6.426450 5.449682

16 17 18 19 20

16 N 0.000000

17 C 1.363675 0.000000

18 N 2.411706 3.518537 0.000000

19 N 2.850087 4.199730 2.434170 0.000000

20 C 2.931698 4.254607 1.361050 1.351006 0.000000

21 C 4.400673 5.716523 2.502018 2.284234 1.469209

22 C 4.986990 6.349921 3.587277 2.280677 2.280369

23 C 4.204451 5.541371 3.545737 1.367046 2.221318

24 N 5.018303 6.267163 4.807236 2.428661 3.531974

25 Zn 2.004043 3.002690 3.374936 2.013001 2.993769

26 C 6.450209 6.100552 8.697806 7.524677 8.565720

27 H 5.073165 4.164154 7.483687 7.183339 7.826310

28 C 7.545424 8.601418 7.790708 5.362000 6.558086

29 H 7.174225 7.833412 8.317390 6.048446 7.399214

30 C 3.734799 2.626342 4.993499 6.496390 6.145452

31 H 3.323923 3.339991 2.843768 5.099632 4.202682

32 C 5.353559 6.561171 3.059732 3.703646 2.605217

33 H 6.064727 7.428167 4.610898 3.315048 3.340619

34 H 7.009886 6.464375 9.344149 8.374868 9.337495

35 H 6.869353 6.624739 9.032983 7.710734 8.809071

36 H 6.869353 6.624739 9.032983 7.710734 8.809071

37 H 7.722308 8.835589 7.763632 5.385997 6.493760

38 H 7.722308 8.835589 7.763632 5.385997 6.493760

39 H 8.397707 9.375689 8.804645 6.370552 7.600882

40 H 4.121477 2.924537 5.576258 6.905333 6.659177

41 H 4.121477 2.924537 5.576258 6.905333 6.659177

42 H 4.456442 3.532384 5.254293 7.061827 6.519270

43 H 5.387826 6.506108 3.061031 4.102833 2.917172

44 H 5.387826 6.506108 3.061031 4.102833 2.917172

45 H 6.360264 7.602845 4.126301 4.418712 3.506505

21 22 23 24 25

21 C 0.000000

22 C 1.375417 0.000000

23 C 2.269282 1.442656 0.000000

24 N 3.576963 2.485839 1.355968 0.000000

25 Zn 4.245955 4.244946 3.023624 3.389605 0.000000

26 C 9.802018 9.568170 8.159516 7.759648 5.578235

27 H 9.254625 9.452762 8.230431 8.326949 5.219461

28 C 6.550852 5.308378 4.393766 3.040272 5.605790

29 H 7.956948 7.029494 5.707683 4.560092 5.219463

30 C 7.482805 8.408926 7.863154 8.751306 5.605790

31 H 5.218125 6.411781 6.339759 7.527948 5.219463

32 C 1.486642 2.592810 3.733673 5.000012 5.578235

33 H 2.212177 1.081653 2.242801 2.850668 5.219461

34 H 10.631643 10.485682 9.098959 8.773784 6.385886

35 H 9.983392 9.661750 8.241041 7.739554 5.838849

36 H 9.983392 9.661750 8.241041 7.739554 5.838849

37 H 6.347034 5.067089 4.316035 3.037796 5.856118

38 H 6.347034 5.067089 4.316035 3.037796 5.856118

39 H 7.637874 6.400016 5.462169 4.106219 6.416735

40 H 8.022447 8.885493 8.261034 9.074077 5.856118

41 H 8.022447 8.885493 8.261034 9.074077 5.856118

42 H 7.750362 8.799313 8.414172 9.405679 6.416735

43 H 2.138330 3.297579 4.307453 5.591285 5.838849

44 H 2.138330 3.297579 4.307453 5.591285 5.838849

45 H 2.140914 2.765626 4.129484 5.249634 6.385886

26 27 28 29 30

26 C 0.000000

27 H 3.008022 0.000000

28 C 7.916858 9.481501 0.000000

29 H 5.261300 7.403294 2.999289 0.000000

30 C 7.899780 5.237983 11.211581 10.408632 0.000000

31 H 9.435980 7.359509 10.408632 10.438927 2.999289

32 C 11.156470 10.376452 7.899780 9.435980 7.916858

33 H 10.376452 10.438922 5.237983 7.359509 9.481501

34 H 1.091889 2.764504 9.008638 6.334896 7.953194

35 H 1.095854 3.758174 7.653470 4.917177 8.512254

36 H 1.095854 3.758174 7.653470 4.917177 8.512254

37 H 8.521229 9.959211 1.095115 3.746794 11.412219

38 H 8.521229 9.959211 1.095115 3.746794 11.412219

39 H 7.983616 9.849452 1.091638 2.770360 12.000295

40 H 7.629568 4.887526 11.412219 10.442000 1.095115

41 H 7.629568 4.887526 11.412219 10.442000 1.095115

42 H 8.991344 6.310533 12.000295 11.364844 1.091638

43 H 11.367358 10.418541 8.512254 9.924277 7.653470

44 H 11.367358 10.418541 8.512254 9.924277 7.653470

45 H 11.941536 11.331468 7.953194 9.793558 9.008638

31 32 33 34 35

31 H 0.000000

32 C 5.261300 0.000000

33 H 7.403294 3.008022 0.000000

34 H 9.793558 11.941536 11.331468 0.000000

35 H 9.924277 11.367358 10.418541 1.772764 0.000000

36 H 9.924277 11.367358 10.418541 1.772764 1.762699

37 H 10.442000 7.629568 4.887526 9.606433 8.183653

38 H 10.442000 7.629568 4.887526 9.606433 8.371294

39 H 11.364844 8.991344 6.310533 9.068356 7.643502

40 H 3.746794 8.521229 9.959211 7.606824 8.166639

41 H 3.746794 8.521229 9.959211 7.606824 8.354662

42 H 2.770360 7.983616 9.849452 9.037311 9.597404

43 H 4.917177 1.095854 3.758174 12.107878 11.543895

44 H 4.917177 1.095854 3.758174 12.107878 11.677698

45 H 6.334896 1.091889 2.764504 12.771773 12.107878

36 37 38 39 40

36 H 0.000000

37 H 8.371294 0.000000

38 H 8.183653 1.762293 0.000000

39 H 7.643502 1.775255 1.775255 0.000000

40 H 8.354662 11.578895 11.712237 12.156714 0.000000

41 H 8.166639 11.712237 11.578895 12.156714 1.762293

42 H 9.597404 12.156714 12.156714 12.833470 1.775255

43 H 11.677698 8.166639 8.354662 9.597404 8.183653

44 H 11.543895 8.354662 8.166639 9.597404 8.371294

45 H 12.107878 7.606824 7.606824 9.037311 9.606433

41 42 43 44 45

41 H 0.000000

42 H 1.775255 0.000000

43 H 8.371294 7.643502 0.000000

44 H 8.183653 7.643502 1.762699 0.000000

45 H 9.606433 9.068356 1.772764 1.772764 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=0 Diff= 2.67D-03

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 2.805557 -1.127452 0.000000

2 7 0 2.012955 -0.013631 0.000000

3 6 0 2.786806 1.093786 0.000000

4 6 0 4.193039 0.668247 0.000000

5 6 0 4.185631 -0.707149 0.000000

6 7 0 2.380187 2.392678 0.000000

7 6 0 1.116557 2.786566 0.000000

8 7 0 0.000000 2.004043 0.000000

9 6 0 -1.116123 2.787547 0.000000

10 6 0 -0.681989 4.221370 0.000000

11 6 0 0.672508 4.198951 0.000000

12 7 0 2.378935 -2.414558 0.000000

13 6 0 0.681989 -4.221370 0.000000

14 6 0 -0.672508 -4.198951 0.000000

15 6 0 -1.116557 -2.786566 0.000000

16 7 0 -0.000000 -2.004043 0.000000

17 6 0 1.116123 -2.787547 0.000000

18 7 0 -2.380187 -2.392678 0.000000

19 7 0 -2.012955 0.013631 0.000000

20 6 0 -2.786806 -1.093786 0.000000

21 6 0 -4.193039 -0.668247 0.000000

22 6 0 -4.185631 0.707149 0.000000

23 6 0 -2.805557 1.127452 0.000000

24 7 0 -2.378935 2.414558 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 5.339390 1.614811 0.000000

27 1 0 5.034353 -1.377704 0.000000

28 6 0 -1.634372 5.362249 0.000000

29 1 0 1.347818 5.042438 0.000000

30 6 0 1.634372 -5.362249 0.000000

31 1 0 -1.347818 -5.042438 0.000000

32 6 0 -5.339390 -1.614811 0.000000

33 1 0 -5.034353 1.377704 0.000000

34 1 0 6.293295 1.083503 0.000000

35 1 0 5.308825 2.265339 0.881350

36 1 0 5.308825 2.265339 -0.881350

37 1 0 -2.283284 5.320180 0.881146

38 1 0 -2.283284 5.320180 -0.881146

39 1 0 -1.110417 6.319926 0.000000

40 1 0 2.283284 -5.320180 0.881146

41 1 0 2.283284 -5.320180 -0.881146

42 1 0 1.110417 -6.319926 0.000000

43 1 0 -5.308825 -2.265339 0.881350

44 1 0 -5.308825 -2.265339 -0.881350

45 1 0 -6.293295 -1.083503 0.000000

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

Rotational constants (GHZ): 0.1839026 0.1816740 0.0915982

Leave Link 202 at Tue Sep 17 14:19:40 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 101 beta electrons

nuclear repulsion energy 2764.1017879655 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= -0.1143459869 Hartrees.

Nuclear repulsion after empirical dispersion term = 2763.9874419786 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 = 3490

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.23D-08

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 128

GePol: Fraction of low-weight points (<1% of avg) = 3.67%

GePol: Cavity surface area = 381.894 Ang\*\*2

GePol: Cavity volume = 379.384 Ang\*\*3

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

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PCM non-electrostatic energy = -0.0108249679 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2763.9766170107 Hartrees.

Leave Link 301 at Tue Sep 17 14:19:40 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= 15353 LenP2D= 41306.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.85D-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 14:19:41 2019, MaxMem= 2415919104 cpu: 12.5

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:19:41 2019, MaxMem= 2415919104 cpu: 1.2

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= -0.000000 -0.000000 0.000000

Rot= 0.999999 0.000000 -0.000000 0.001233 Ang= 0.14 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)

(BU) (AG) (BU) (AG) (BU) (AG) (BU) (AG) (BU) (AG)

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(AG) (AG) (BU) (BU) (BG) (BG) (AG) (AG) (BU) (BU)

(AG) (BU) (BU) (AG) (AG) (AU) (BG) (BG) (AG) (BU)

(AU) (BU) (AG) (AU) (BG) (BG) (AG) (AG) (AU) (BU)

(BU) (AU) (AG) (BU) (BU) (AG) (AG) (BG) (BU) (BU)

(BG) (AG) (BU) (BU) (AU) (AG) (BG) (AG) (AU) (AU)

(BG) (AU) (BG)

Virtual (AG) (AG) (AG) (AG) (AG) (AG) (AG) (AG) (AG) (AG)

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The electronic state of the initial guess is 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0178 S= 1.0059

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= -1276.14897243770

Leave Link 401 at Tue Sep 17 14:19:43 2019, MaxMem= 2415919104 cpu: 38.9

(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= 36540300.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.44D-15 for 3486.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.79D-15 for 1770 729.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.99D-15 for 3486.

Iteration 1 A^-1\*A deviation from orthogonality is 4.99D-13 for 1981 1967.

E= -1275.84130883388

DIIS: error= 6.03D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.84130883388 IErMin= 1 ErrMin= 6.03D-04

ErrMax= 6.03D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.75D-03 BMatP= 1.75D-03

IDIUse=3 WtCom= 9.94D-01 WtEn= 6.03D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.302 Goal= None Shift= 0.000

Gap= 0.393 Goal= None Shift= 0.000

RMSDP=7.44D-05 MaxDP=1.91D-03 OVMax= 1.01D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 7.44D-05 CP: 1.00D+00

E= -1275.84187917422 Delta-E= -0.000570340345 Rises=F Damp=F

DIIS: error= 3.06D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84187917422 IErMin= 2 ErrMin= 3.06D-04

ErrMax= 3.06D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.68D-04 BMatP= 1.75D-03

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.06D-03

Coeff-Com: 0.106D+00 0.894D+00

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

Coeff: 0.106D+00 0.894D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.16D-05 MaxDP=9.93D-04 DE=-5.70D-04 OVMax= 7.11D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.13D-05 CP: 1.00D+00 1.04D+00

E= -1275.84186405750 Delta-E= 0.000015116719 Rises=F Damp=F

DIIS: error= 4.71D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1275.84187917422 IErMin= 2 ErrMin= 3.06D-04

ErrMax= 4.71D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.83D-04 BMatP= 1.68D-04

IDIUse=3 WtCom= 3.15D-01 WtEn= 6.85D-01

Coeff-Com: -0.127D-01 0.574D+00 0.439D+00

Coeff-En: 0.000D+00 0.570D+00 0.430D+00

Coeff: -0.400D-02 0.571D+00 0.433D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=1.29D-05 MaxDP=5.87D-04 DE= 1.51D-05 OVMax= 2.86D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 9.02D-06 CP: 1.00D+00 1.06D+00 5.76D-01

E= -1275.84192736362 Delta-E= -0.000063306116 Rises=F Damp=F

DIIS: error= 1.03D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84192736362 IErMin= 4 ErrMin= 1.03D-04

ErrMax= 1.03D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.01D-06 BMatP= 1.68D-04

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.03D-03

Coeff-Com: -0.113D-01 0.173D+00 0.200D+00 0.638D+00

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

Coeff: -0.113D-01 0.173D+00 0.200D+00 0.638D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=5.29D-06 MaxDP=3.10D-04 DE=-6.33D-05 OVMax= 3.61D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.03D-06 CP: 1.00D+00 1.08D+00 6.81D-01 1.26D+00

E= -1275.84193206752 Delta-E= -0.000004703899 Rises=F Damp=F

DIIS: error= 8.22D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84193206752 IErMin= 5 ErrMin= 8.22D-05

ErrMax= 8.22D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.66D-06 BMatP= 9.01D-06

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

Coeff-Com: -0.397D-02 0.278D-01 0.637D-01 0.374D+00 0.538D+00

Coeff: -0.397D-02 0.278D-01 0.637D-01 0.374D+00 0.538D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=3.60D-06 MaxDP=1.66D-04 DE=-4.70D-06 OVMax= 2.60D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.55D-06 CP: 1.00D+00 1.09D+00 7.46D-01 1.55D+00 1.27D+00

E= -1275.84193457769 Delta-E= -0.000002510176 Rises=F Damp=F

DIIS: error= 7.58D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84193457769 IErMin= 6 ErrMin= 7.58D-05

ErrMax= 7.58D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.97D-07 BMatP= 2.66D-06

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

Coeff-Com: 0.376D-02-0.636D-01-0.571D-01-0.879D-01 0.677D-01 0.114D+01

Coeff: 0.376D-02-0.636D-01-0.571D-01-0.879D-01 0.677D-01 0.114D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=6.78D-06 MaxDP=3.49D-04 DE=-2.51D-06 OVMax= 5.22D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.25D-06 CP: 1.00D+00 1.10D+00 8.69D-01 2.09D+00 2.07D+00

CP: 2.00D+00

E= -1275.84193789062 Delta-E= -0.000003312925 Rises=F Damp=F

DIIS: error= 5.45D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84193789062 IErMin= 7 ErrMin= 5.45D-05

ErrMax= 5.45D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.18D-07 BMatP= 7.97D-07

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

Coeff-Com: 0.502D-02-0.613D-01-0.806D-01-0.281D+00-0.393D+00 0.836D+00

Coeff-Com: 0.975D+00

Coeff: 0.502D-02-0.613D-01-0.806D-01-0.281D+00-0.393D+00 0.836D+00

Coeff: 0.975D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=8.03D-06 MaxDP=3.99D-04 DE=-3.31D-06 OVMax= 6.17D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.14D-06 CP: 1.00D+00 1.12D+00 1.00D+00 2.72D+00 3.00D+00

CP: 3.00D+00 1.85D+00

E= -1275.84194066961 Delta-E= -0.000002778994 Rises=F Damp=F

DIIS: error= 3.74D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84194066961 IErMin= 8 ErrMin= 3.74D-05

ErrMax= 3.74D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.29D-07 BMatP= 7.18D-07

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

Coeff-Com: 0.609D-05 0.192D-01 0.364D-02-0.446D-01-0.271D+00-0.310D+00

Coeff-Com: 0.408D+00 0.119D+01

Coeff: 0.609D-05 0.192D-01 0.364D-02-0.446D-01-0.271D+00-0.310D+00

Coeff: 0.408D+00 0.119D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=7.69D-06 MaxDP=3.95D-04 DE=-2.78D-06 OVMax= 6.02D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 4.81D-06 CP: 1.00D+00 1.14D+00 1.13D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.99D+00

E= -1275.84194208697 Delta-E= -0.000001417362 Rises=F Damp=F

DIIS: error= 1.83D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84194208697 IErMin= 9 ErrMin= 1.83D-05

ErrMax= 1.83D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.37D-07 BMatP= 2.29D-07

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

Coeff-Com: -0.187D-02 0.346D-01 0.314D-01 0.765D-01-0.377D-01-0.479D+00

Coeff-Com: -0.115D+00 0.766D+00 0.724D+00

Coeff: -0.187D-02 0.346D-01 0.314D-01 0.765D-01-0.377D-01-0.479D+00

Coeff: -0.115D+00 0.766D+00 0.724D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=3.40D-06 MaxDP=1.69D-04 DE=-1.42D-06 OVMax= 2.63D-03

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.77D-06 CP: 1.00D+00 1.15D+00 1.18D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.54D+00

E= -1275.84194238123 Delta-E= -0.000000294255 Rises=F Damp=F

DIIS: error= 9.65D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84194238123 IErMin=10 ErrMin= 9.65D-06

ErrMax= 9.65D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.47D-08 BMatP= 1.37D-07

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

Coeff-Com: -0.997D-03 0.126D-01 0.171D-01 0.679D-01 0.899D-01-0.154D+00

Coeff-Com: -0.238D+00 0.118D-01 0.425D+00 0.769D+00

Coeff: -0.997D-03 0.126D-01 0.171D-01 0.679D-01 0.899D-01-0.154D+00

Coeff: -0.238D+00 0.118D-01 0.425D+00 0.769D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=1.24D-06 MaxDP=6.89D-05 DE=-2.94D-07 OVMax= 9.70D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 3.48D-07 CP: 1.00D+00 1.15D+00 1.20D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.74D+00 1.34D+00

E= -1275.84194243862 Delta-E= -0.000000057396 Rises=F Damp=F

DIIS: error= 4.34D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84194243862 IErMin=11 ErrMin= 4.34D-06

ErrMax= 4.34D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.20D-08 BMatP= 3.47D-08

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

Coeff-Com: -0.474D-04-0.293D-02-0.755D-04 0.151D-01 0.531D-01 0.476D-01

Coeff-Com: -0.101D+00-0.191D+00-0.423D-02 0.439D+00 0.744D+00

Coeff: -0.474D-04-0.293D-02-0.755D-04 0.151D-01 0.531D-01 0.476D-01

Coeff: -0.101D+00-0.191D+00-0.423D-02 0.439D+00 0.744D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=7.49D-07 MaxDP=3.71D-05 DE=-5.74D-08 OVMax= 5.79D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.28D-07 CP: 1.00D+00 1.15D+00 1.21D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.85D+00 1.56D+00

CP: 1.22D+00

E= -1275.84194245578 Delta-E= -0.000000017152 Rises=F Damp=F

DIIS: error= 1.77D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84194245578 IErMin=12 ErrMin= 1.77D-06

ErrMax= 1.77D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.31D-09 BMatP= 1.20D-08

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

Coeff-Com: 0.180D-03-0.405D-02-0.383D-02-0.537D-02 0.639D-02 0.573D-01

Coeff-Com: -0.579D-02-0.878D-01-0.101D+00 0.960D-01 0.310D+00 0.738D+00

Coeff: 0.180D-03-0.405D-02-0.383D-02-0.537D-02 0.639D-02 0.573D-01

Coeff: -0.579D-02-0.878D-01-0.101D+00 0.960D-01 0.310D+00 0.738D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=2.28D-07 MaxDP=1.23D-05 DE=-1.72D-08 OVMax= 1.75D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 6.36D-08 CP: 1.00D+00 1.15D+00 1.21D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.89D+00 1.63D+00

CP: 1.37D+00 1.20D+00

E= -1275.84194245879 Delta-E= -0.000000003017 Rises=F Damp=F

DIIS: error= 1.25D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84194245879 IErMin=13 ErrMin= 1.25D-06

ErrMax= 1.25D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.45D-09 BMatP= 2.31D-09

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

Coeff-Com: 0.144D-03-0.145D-02-0.263D-02-0.902D-02-0.174D-01 0.171D-01

Coeff-Com: 0.332D-01 0.220D-01-0.749D-01-0.101D+00-0.142D+00 0.519D+00

Coeff-Com: 0.757D+00

Coeff: 0.144D-03-0.145D-02-0.263D-02-0.902D-02-0.174D-01 0.171D-01

Coeff: 0.332D-01 0.220D-01-0.749D-01-0.101D+00-0.142D+00 0.519D+00

Coeff: 0.757D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=2.46D-07 MaxDP=1.21D-05 DE=-3.02D-09 OVMax= 1.88D-04

Cycle 14 Pass 1 IDiag 1:

RMSU= 3.93D-08 CP: 1.00D+00 1.15D+00 1.22D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.92D+00 1.70D+00

CP: 1.45D+00 1.57D+00 1.24D+00

E= -1275.84194246054 Delta-E= -0.000000001744 Rises=F Damp=F

DIIS: error= 4.25D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84194246054 IErMin=14 ErrMin= 4.25D-07

ErrMax= 4.25D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.81D-10 BMatP= 1.45D-09

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

Coeff-Com: -0.161D-05 0.836D-03 0.218D-03-0.165D-02-0.968D-02-0.138D-01

Coeff-Com: 0.161D-01 0.419D-01 0.275D-02-0.694D-01-0.181D+00-0.468D-02

Coeff-Com: 0.313D+00 0.905D+00

Coeff: -0.161D-05 0.836D-03 0.218D-03-0.165D-02-0.968D-02-0.138D-01

Coeff: 0.161D-01 0.419D-01 0.275D-02-0.694D-01-0.181D+00-0.468D-02

Coeff: 0.313D+00 0.905D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=9.23D-08 MaxDP=4.78D-06 DE=-1.74D-09 OVMax= 6.86D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 1.54D-08 CP: 1.00D+00 1.15D+00 1.22D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.94D+00 1.72D+00

CP: 1.50D+00 1.74D+00 1.58D+00 1.33D+00

E= -1275.84194246080 Delta-E= -0.000000000261 Rises=F Damp=F

DIIS: error= 1.94D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.84194246080 IErMin=15 ErrMin= 1.94D-07

ErrMax= 1.94D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.49D-11 BMatP= 1.81D-10

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

Coeff-Com: -0.269D-04 0.689D-03 0.599D-03 0.749D-03-0.159D-02-0.109D-01

Coeff-Com: 0.241D-02 0.169D-01 0.164D-01-0.180D-01-0.654D-01-0.104D+00

Coeff-Com: 0.165D-01 0.483D+00 0.663D+00

Coeff: -0.269D-04 0.689D-03 0.599D-03 0.749D-03-0.159D-02-0.109D-01

Coeff: 0.241D-02 0.169D-01 0.164D-01-0.180D-01-0.654D-01-0.104D+00

Coeff: 0.165D-01 0.483D+00 0.663D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=3.00D-08 MaxDP=1.60D-06 DE=-2.61D-10 OVMax= 2.16D-05

Cycle 16 Pass 1 IDiag 1:

RMSU= 7.06D-09 CP: 1.00D+00 1.15D+00 1.22D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.94D+00 1.73D+00

CP: 1.51D+00 1.80D+00 1.67D+00 1.49D+00 1.08D+00

E= -1275.84194246082 Delta-E= -0.000000000026 Rises=F Damp=F

DIIS: error= 1.06D-07 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1275.84194246082 IErMin=16 ErrMin= 1.06D-07

ErrMax= 1.06D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.41D-12 BMatP= 5.49D-11

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

Coeff-Com: -0.106D-04 0.127D-03 0.206D-03 0.622D-03 0.138D-02-0.168D-02

Coeff-Com: -0.159D-02-0.153D-02 0.701D-02 0.471D-02 0.898D-02-0.440D-01

Coeff-Com: -0.490D-01 0.273D-01 0.275D+00 0.773D+00

Coeff: -0.106D-04 0.127D-03 0.206D-03 0.622D-03 0.138D-02-0.168D-02

Coeff: -0.159D-02-0.153D-02 0.701D-02 0.471D-02 0.898D-02-0.440D-01

Coeff: -0.490D-01 0.273D-01 0.275D+00 0.773D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=1.54D-08 MaxDP=6.95D-07 DE=-2.59D-11 OVMax= 1.12D-05

Cycle 17 Pass 1 IDiag 1:

RMSU= 3.86D-09 CP: 1.00D+00 1.15D+00 1.22D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.94D+00 1.73D+00

CP: 1.52D+00 1.81D+00 1.70D+00 1.53D+00 1.21D+00

CP: 1.09D+00

E= -1275.84194246085 Delta-E= -0.000000000023 Rises=F Damp=F

DIIS: error= 6.54D-08 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=17 EnMin= -1275.84194246085 IErMin=17 ErrMin= 6.54D-08

ErrMax= 6.54D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.15D-12 BMatP= 9.41D-12

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

Coeff-Com: 0.686D-06-0.105D-03-0.394D-04 0.145D-03 0.128D-02 0.185D-02

Coeff-Com: -0.152D-02-0.551D-02 0.188D-03 0.728D-02 0.237D-01-0.593D-03

Coeff-Com: -0.331D-01-0.111D+00-0.130D-02 0.463D+00 0.656D+00

Coeff: 0.686D-06-0.105D-03-0.394D-04 0.145D-03 0.128D-02 0.185D-02

Coeff: -0.152D-02-0.551D-02 0.188D-03 0.728D-02 0.237D-01-0.593D-03

Coeff: -0.331D-01-0.111D+00-0.130D-02 0.463D+00 0.656D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=6.60D-09 MaxDP=2.90D-07 DE=-2.32D-11 OVMax= 4.89D-06

Error on total polarization charges = 0.06470

SCF Done: E(UB3LYP) = -1275.84194246 A.U. after 17 cycles

NFock= 17 Conv=0.66D-08 -V/T= 1.9659

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0183 S= 1.0061

<L.S>= 0.000000000000E+00

KE= 1.320891976918D+03 PE=-8.579965413061D+03 EE= 3.219254876671D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.79

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0183, after 2.0002

Leave Link 502 at Tue Sep 17 14:21:11 2019, MaxMem= 2415919104 cpu: 1548.2

(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= 15353 LenP2D= 41306.

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 = 246

Leave Link 701 at Tue Sep 17 14:21:15 2019, MaxMem= 2415919104 cpu: 68.7

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 14:21:15 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 14:21:25 2019, MaxMem= 2415919104 cpu: 177.9

(Enter /home/blab/g09/l716.exe)

Dipole = 7.99360578D-14-4.88498131D-15 0.00000000D+00

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.003949184 -0.003580890 0.000000000

2 7 0.002828831 0.003997879 -0.000000000

3 6 -0.004902982 0.000377448 -0.000000000

4 6 0.000894604 -0.002312044 -0.000000000

5 6 0.001977119 -0.000855471 -0.000000000

6 7 0.005338404 -0.001101719 0.000000000

7 6 -0.001315456 0.000730306 -0.000000000

8 7 -0.003122387 0.000552673 0.000000000

9 6 -0.000247119 0.002141067 0.000000000

10 6 -0.003119232 -0.005181503 0.000000000

11 6 0.004532504 0.001213413 -0.000000000

12 7 -0.006704921 0.005124206 -0.000000000

13 6 0.003119232 0.005181503 0.000000000

14 6 -0.004532504 -0.001213413 0.000000000

15 6 0.001315456 -0.000730306 0.000000000

16 7 0.003122387 -0.000552673 0.000000000

17 6 0.000247119 -0.002141067 0.000000000

18 7 -0.005338404 0.001101719 0.000000000

19 7 -0.002828831 -0.003997879 -0.000000000

20 6 0.004902982 -0.000377448 -0.000000000

21 6 -0.000894604 0.002312044 -0.000000000

22 6 -0.001977119 0.000855471 -0.000000000

23 6 -0.003949184 0.003580890 -0.000000000

24 7 0.006704921 -0.005124206 0.000000000

25 30 -0.000000000 -0.000000000 0.000000000

26 6 -0.001430910 -0.001118890 0.000000000

27 1 0.000791560 -0.000423930 0.000000000

28 6 -0.000584567 -0.001822521 -0.000000000

29 1 0.000496076 -0.000507871 -0.000000000

30 6 0.000584567 0.001822521 0.000000000

31 1 -0.000496076 0.000507871 -0.000000000

32 6 0.001430910 0.001118890 0.000000000

33 1 -0.000791560 0.000423930 -0.000000000

34 1 0.000310787 -0.000046614 -0.000000000

35 1 0.000323064 -0.000455477 -0.000983629

36 1 0.000323064 -0.000455477 0.000983629

37 1 0.000345205 0.000367280 -0.000878133

38 1 0.000345205 0.000367280 0.000878133

39 1 -0.000281745 0.000290560 -0.000000000

40 1 -0.000345205 -0.000367280 -0.000878133

41 1 -0.000345205 -0.000367280 0.000878133

42 1 0.000281745 -0.000290560 0.000000000

43 1 -0.000323064 0.000455477 -0.000983629

44 1 -0.000323064 0.000455477 0.000983629

45 1 -0.000310787 0.000046614 -0.000000000

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

Cartesian Forces: Max 0.006704921 RMS 0.002025761

Leave Link 716 at Tue Sep 17 14:21:25 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 0.008846946 RMS 0.001265812

Search for a local minimum.

Step number 18 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 12 13 14 15

16 17 18

DE= 7.34D-04 DEPred=-2.99D-05 R=-2.45D+01

Trust test=-2.45D+01 RLast= 8.08D-02 DXMaxT set to 5.00D-02

ITU= -1 -1 1 1 -1 1 1 1 -1 0 1 -1 1 1 1 1 0 0

Eigenvalues --- 0.00284 0.00878 0.00878 0.00878 0.00878

Eigenvalues --- 0.01344 0.01346 0.01348 0.01348 0.01605

Eigenvalues --- 0.01623 0.01633 0.01639 0.01776 0.01793

Eigenvalues --- 0.01814 0.01822 0.01891 0.01908 0.01940

Eigenvalues --- 0.01948 0.01999 0.02000 0.02045 0.02048

Eigenvalues --- 0.02070 0.02089 0.02104 0.02112 0.02115

Eigenvalues --- 0.02206 0.02314 0.02317 0.02352 0.02374

Eigenvalues --- 0.04233 0.07234 0.07234 0.07239 0.07239

Eigenvalues --- 0.07353 0.07420 0.07429 0.07465 0.10818

Eigenvalues --- 0.14492 0.14504 0.15273 0.15518 0.15705

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16020 0.16072 0.16170 0.16637 0.20237

Eigenvalues --- 0.21918 0.22075 0.22102 0.23808 0.23843

Eigenvalues --- 0.23856 0.24322 0.24792 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25033

Eigenvalues --- 0.26322 0.28549 0.29536 0.31024 0.32266

Eigenvalues --- 0.32912 0.33188 0.33203 0.33282 0.33282

Eigenvalues --- 0.33535 0.33718 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33724 0.33724 0.34358 0.34410

Eigenvalues --- 0.34437 0.34437 0.34500 0.35439 0.35557

Eigenvalues --- 0.35559 0.35592 0.35682 0.35682 0.36185

Eigenvalues --- 0.37977 0.38375 0.41626 0.41801 0.43949

Eigenvalues --- 0.44904 0.47652 0.48967 0.48988 0.51351

Eigenvalues --- 0.51364 0.51956 0.52310 0.53643 0.54000

Eigenvalues --- 0.54011 0.56163 0.56329 0.56332

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 0.02307 0.85069 0.12623

Cosine: 1.000 > 0.840

Length: 0.999

GDIIS step was calculated using 3 of the last 18 vectors.

Maximum step size ( 0.050) exceeded in Quadratic search.

-- Step size scaled by 0.626

Iteration 1 RMS(Cart)= 0.00946004 RMS(Int)= 0.00001920

Iteration 2 RMS(Cart)= 0.00002801 RMS(Int)= 0.00000172

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000172

ITry= 1 IFail=0 DXMaxC= 4.25D-02 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 6.11D-10 for atom 33.

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

(Linear) (Quad) (Total)

R1 2.58334 0.00116 -0.00066 0.00094 0.00028 2.58362

R2 2.72623 0.00285 0.00328 0.00141 0.00469 2.73091

R3 2.56241 0.00885 0.01531 -0.00066 0.01464 2.57705

R4 2.55303 0.00262 0.00512 -0.00034 0.00478 2.55781

R5 3.80402 -0.00046 -0.00270 0.00189 -0.00081 3.80321

R6 2.77640 0.00106 -0.00183 0.00051 -0.00132 2.77508

R7 2.57201 0.00286 0.00536 -0.00185 0.00351 2.57553

R8 2.59916 -0.00050 -0.00056 -0.00066 -0.00122 2.59794

R9 2.80935 0.00183 0.00237 0.00138 0.00375 2.81310

R10 2.04403 -0.00047 -0.00063 -0.00038 -0.00101 2.04302

R11 2.50123 -0.00165 -0.00250 0.00337 0.00086 2.50209

R12 2.57658 0.00203 0.00348 -0.00097 0.00251 2.57909

R13 2.79782 0.00094 0.00200 -0.00166 0.00034 2.79816

R14 2.57697 0.00082 0.00092 0.00082 0.00174 2.57871

R15 3.78709 0.00015 -0.00251 0.00320 0.00069 3.78778

R16 2.83101 0.00256 0.00628 -0.00235 0.00393 2.83494

R17 2.48828 0.00087 -0.00066 0.00340 0.00274 2.49102

R18 2.55998 -0.00450 -0.00629 0.00132 -0.00496 2.55502

R19 2.80841 -0.00042 -0.00099 -0.00039 -0.00137 2.80704

R20 2.04188 0.00069 0.00090 0.00075 0.00165 2.04353

R21 2.48828 0.00087 -0.00066 0.00340 0.00274 2.49102

R22 2.55998 -0.00450 -0.00629 0.00132 -0.00496 2.55502

R23 2.83101 0.00256 0.00628 -0.00235 0.00393 2.83494

R24 2.80841 -0.00042 -0.00099 -0.00039 -0.00137 2.80704

R25 2.79782 0.00094 0.00200 -0.00166 0.00034 2.79816

R26 2.04188 0.00069 0.00090 0.00075 0.00165 2.04353

R27 2.57658 0.00203 0.00348 -0.00097 0.00251 2.57909

R28 2.50123 -0.00165 -0.00250 0.00337 0.00086 2.50209

R29 2.57697 0.00082 0.00092 0.00082 0.00174 2.57871

R30 3.78709 0.00015 -0.00251 0.00320 0.00069 3.78778

R31 2.57201 0.00286 0.00536 -0.00185 0.00351 2.57553

R32 2.55303 0.00262 0.00512 -0.00034 0.00478 2.55781

R33 2.58334 0.00116 -0.00066 0.00094 0.00028 2.58362

R34 3.80402 -0.00046 -0.00270 0.00189 -0.00081 3.80321

R35 2.77640 0.00106 -0.00183 0.00051 -0.00132 2.77508

R36 2.59916 -0.00050 -0.00056 -0.00066 -0.00122 2.59794

R37 2.80935 0.00183 0.00237 0.00138 0.00375 2.81310

R38 2.72623 0.00285 0.00328 0.00141 0.00469 2.73091

R39 2.04403 -0.00047 -0.00063 -0.00038 -0.00101 2.04302

R40 2.56241 0.00885 0.01531 -0.00066 0.01464 2.57705

R41 2.06337 -0.00021 -0.00061 0.00006 -0.00054 2.06283

R42 2.07086 -0.00052 -0.00081 0.00015 -0.00067 2.07020

R43 2.07086 -0.00052 -0.00081 0.00015 -0.00067 2.07020

R44 2.06947 -0.00044 -0.00046 -0.00005 -0.00051 2.06896

R45 2.06947 -0.00044 -0.00046 -0.00005 -0.00051 2.06896

R46 2.06290 -0.00040 -0.00082 -0.00009 -0.00091 2.06199

R47 2.06947 -0.00044 -0.00046 -0.00005 -0.00051 2.06896

R48 2.06947 -0.00044 -0.00046 -0.00005 -0.00051 2.06896

R49 2.06290 -0.00040 -0.00082 -0.00009 -0.00091 2.06199

R50 2.07086 -0.00052 -0.00081 0.00015 -0.00067 2.07020

R51 2.07086 -0.00052 -0.00081 0.00015 -0.00067 2.07020

R52 2.06337 -0.00021 -0.00061 0.00006 -0.00054 2.06283

A1 1.89364 -0.00089 -0.00103 -0.00109 -0.00212 1.89153

A2 2.20306 -0.00060 0.00090 0.00034 0.00124 2.20429

A3 2.18649 0.00149 0.00013 0.00075 0.00088 2.18737

A4 1.91321 -0.00140 -0.00356 0.00035 -0.00321 1.90999

A5 2.19604 -0.00025 -0.00282 -0.00089 -0.00372 2.19232

A6 2.17394 0.00165 0.00638 0.00054 0.00693 2.18087

A7 1.88686 0.00211 0.00510 0.00031 0.00540 1.89226

A8 2.22829 -0.00068 -0.00275 -0.00029 -0.00304 2.22526

A9 2.16803 -0.00143 -0.00235 -0.00002 -0.00237 2.16566

A10 1.85926 -0.00199 -0.00459 -0.00030 -0.00489 1.85437

A11 2.15752 0.00268 0.00978 0.00071 0.01049 2.16801

A12 2.26641 -0.00069 -0.00519 -0.00041 -0.00561 2.26080

A13 1.87181 0.00217 0.00408 0.00073 0.00481 1.87662

A14 2.17731 -0.00031 0.00234 -0.00002 0.00231 2.17962

A15 2.23407 -0.00186 -0.00642 -0.00071 -0.00713 2.22694

A16 2.17635 -0.00164 -0.00516 0.00120 -0.00397 2.17238

A17 2.22814 0.00076 0.00205 -0.00105 0.00099 2.22913

A18 2.17757 -0.00249 -0.00571 0.00005 -0.00566 2.17191

A19 1.87747 0.00174 0.00366 0.00100 0.00467 1.88214

A20 1.91825 -0.00178 -0.00209 -0.00053 -0.00263 1.91562

A21 2.18208 0.00131 0.00438 0.00015 0.00453 2.18662

A22 2.18285 0.00047 -0.00229 0.00038 -0.00190 2.18095

A23 1.88885 -0.00111 -0.00312 -0.00007 -0.00319 1.88566

A24 2.24234 0.00011 0.00280 -0.00246 0.00035 2.24268

A25 2.15200 0.00100 0.00031 0.00252 0.00284 2.15484

A26 1.84825 0.00255 0.00530 0.00055 0.00585 1.85410

A27 2.15200 0.00001 0.00142 0.00212 0.00354 2.15553

A28 2.28294 -0.00256 -0.00672 -0.00267 -0.00939 2.27355

A29 1.89196 -0.00140 -0.00375 -0.00095 -0.00470 1.88726

A30 2.16186 0.00088 0.00185 0.00147 0.00332 2.16518

A31 2.22936 0.00051 0.00190 -0.00052 0.00138 2.23075

A32 2.17806 -0.00113 -0.00350 0.00208 -0.00142 2.17664

A33 1.84825 0.00255 0.00530 0.00055 0.00585 1.85410

A34 2.28294 -0.00256 -0.00672 -0.00267 -0.00939 2.27355

A35 2.15200 0.00001 0.00142 0.00212 0.00354 2.15553

A36 1.89196 -0.00140 -0.00375 -0.00095 -0.00470 1.88726

A37 2.22936 0.00051 0.00190 -0.00052 0.00138 2.23075

A38 2.16186 0.00088 0.00185 0.00147 0.00332 2.16518

A39 1.87747 0.00174 0.00366 0.00100 0.00467 1.88214

A40 2.17757 -0.00249 -0.00571 0.00005 -0.00566 2.17191

A41 2.22814 0.00076 0.00205 -0.00105 0.00099 2.22913

A42 1.91825 -0.00178 -0.00209 -0.00053 -0.00263 1.91562

A43 2.18208 0.00131 0.00438 0.00015 0.00453 2.18662

A44 2.18285 0.00047 -0.00229 0.00038 -0.00190 2.18095

A45 2.15200 0.00100 0.00031 0.00252 0.00284 2.15484

A46 2.24234 0.00011 0.00280 -0.00246 0.00035 2.24268

A47 1.88885 -0.00111 -0.00312 -0.00007 -0.00319 1.88566

A48 2.17635 -0.00164 -0.00516 0.00120 -0.00397 2.17238

A49 1.91321 -0.00140 -0.00356 0.00035 -0.00321 1.90999

A50 2.17394 0.00165 0.00638 0.00054 0.00693 2.18087

A51 2.19604 -0.00025 -0.00282 -0.00089 -0.00372 2.19232

A52 2.22829 -0.00068 -0.00275 -0.00029 -0.00304 2.22526

A53 2.16803 -0.00143 -0.00235 -0.00002 -0.00237 2.16566

A54 1.88686 0.00211 0.00510 0.00031 0.00540 1.89226

A55 1.85926 -0.00199 -0.00459 -0.00030 -0.00489 1.85437

A56 2.15752 0.00268 0.00978 0.00071 0.01049 2.16801

A57 2.26641 -0.00069 -0.00519 -0.00041 -0.00561 2.26080

A58 1.87181 0.00217 0.00408 0.00073 0.00481 1.87662

A59 2.23407 -0.00186 -0.00642 -0.00071 -0.00713 2.22694

A60 2.17731 -0.00031 0.00234 -0.00002 0.00231 2.17962

A61 1.89364 -0.00089 -0.00103 -0.00109 -0.00212 1.89153

A62 2.20306 -0.00060 0.00090 0.00034 0.00124 2.20429

A63 2.18649 0.00149 0.00013 0.00075 0.00088 2.18737

A64 2.17806 -0.00113 -0.00350 0.00208 -0.00142 2.17664

A65 1.57757 -0.00140 -0.00491 -0.00055 -0.00545 1.57211

A66 1.56402 0.00140 0.00491 0.00055 0.00545 1.56948

A67 1.56402 0.00140 0.00491 0.00055 0.00545 1.56948

A68 1.57757 -0.00140 -0.00491 -0.00055 -0.00545 1.57211

A69 1.94318 0.00015 -0.00012 -0.00088 -0.00100 1.94218

A70 1.93527 0.00079 0.00332 0.00069 0.00401 1.93929

A71 1.93527 0.00079 0.00332 0.00069 0.00401 1.93929

A72 1.88938 -0.00031 0.00006 -0.00004 0.00003 1.88941

A73 1.88938 -0.00031 0.00006 -0.00004 0.00003 1.88941

A74 1.86885 -0.00123 -0.00705 -0.00045 -0.00750 1.86135

A75 1.92862 0.00071 0.00327 0.00046 0.00373 1.93236

A76 1.92862 0.00071 0.00327 0.00046 0.00373 1.93236

A77 1.94538 -0.00017 -0.00026 -0.00147 -0.00172 1.94366

A78 1.87006 -0.00109 -0.00755 0.00023 -0.00732 1.86274

A79 1.89453 -0.00010 0.00044 0.00019 0.00063 1.89516

A80 1.89453 -0.00010 0.00044 0.00019 0.00063 1.89516

A81 1.92862 0.00071 0.00327 0.00046 0.00373 1.93236

A82 1.92862 0.00071 0.00327 0.00046 0.00373 1.93236

A83 1.94538 -0.00017 -0.00026 -0.00147 -0.00172 1.94366

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A85 1.89453 -0.00010 0.00044 0.00019 0.00063 1.89516

A86 1.89453 -0.00010 0.00044 0.00019 0.00063 1.89516

A87 1.93527 0.00079 0.00332 0.00069 0.00401 1.93929

A88 1.93527 0.00079 0.00332 0.00069 0.00401 1.93929

A89 1.94318 0.00015 -0.00012 -0.00088 -0.00100 1.94218

A90 1.86885 -0.00123 -0.00705 -0.00045 -0.00750 1.86135

A91 1.88938 -0.00031 0.00006 -0.00004 0.00003 1.88941

A92 1.88938 -0.00031 0.00006 -0.00004 0.00003 1.88941

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A96 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

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D4 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

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D6 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

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D9 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

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D14 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

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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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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

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D26 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

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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 1.03685 -0.00025 -0.00226 0.00017 -0.00210 1.03475

D31 -1.03685 0.00025 0.00226 -0.00017 0.00210 -1.03475

D32 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.10475 -0.00025 -0.00226 0.00017 -0.00210 -2.10684

D34 2.10475 0.00025 0.00226 -0.00017 0.00210 2.10684

D35 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

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D45 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

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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 1.03337 -0.00024 -0.00262 0.00043 -0.00219 1.03118

D64 -1.03337 0.00024 0.00262 -0.00043 0.00219 -1.03118

D65 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D66 -2.10823 -0.00024 -0.00262 0.00043 -0.00219 -2.11041

D67 2.10823 0.00024 0.00262 -0.00043 0.00219 2.11041

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

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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 -2.10823 -0.00024 -0.00262 0.00043 -0.00219 -2.11041

D80 2.10823 0.00024 0.00262 -0.00043 0.00219 2.11041

D81 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D82 1.03337 -0.00024 -0.00262 0.00043 -0.00219 1.03118

D83 -1.03337 0.00024 0.00262 -0.00043 0.00219 -1.03118

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

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D106 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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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

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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

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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

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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 1.03685 -0.00025 -0.00226 0.00017 -0.00210 1.03475

D126 -1.03685 0.00025 0.00226 -0.00017 0.00210 -1.03475

D127 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D128 -2.10475 -0.00025 -0.00226 0.00017 -0.00210 -2.10684

D129 2.10475 0.00025 0.00226 -0.00017 0.00210 2.10684

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

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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 0.008847 0.000450 NO

RMS Force 0.001266 0.000300 NO

Maximum Displacement 0.042540 0.001800 NO

RMS Displacement 0.009460 0.001200 NO

Predicted change in Energy=-6.347881D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:21:25 2019, MaxMem= 2415919104 cpu: 1.3

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.078084 -2.192169 0.000000

2 7 0 -0.749970 -1.867617 0.000000

3 6 0 -0.009479 -3.000636 0.000000

4 6 0 -0.921931 -4.151268 0.000000

5 6 0 -2.195093 -3.632561 0.000000

6 7 0 1.349538 -3.103560 0.000000

7 6 0 2.179182 -2.071667 0.000000

8 7 0 1.861023 -0.744475 0.000000

9 6 0 3.002378 0.003475 0.000000

10 6 0 4.172809 -0.934953 0.000000

11 6 0 3.655623 -2.184183 0.000000

12 7 0 -3.123195 -1.316118 0.000000

13 6 0 -4.172809 0.934953 0.000000

14 6 0 -3.655623 2.184183 0.000000

15 6 0 -2.179182 2.071667 0.000000

16 7 0 -1.861023 0.744475 0.000000

17 6 0 -3.002378 -0.003475 0.000000

18 7 0 -1.349538 3.103560 0.000000

19 7 0 0.749970 1.867617 0.000000

20 6 0 0.009479 3.000636 0.000000

21 6 0 0.921931 4.151268 0.000000

22 6 0 2.195093 3.632561 0.000000

23 6 0 2.078084 2.192169 0.000000

24 7 0 3.123195 1.316118 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.477569 -5.572027 0.000000

27 1 0 -3.129109 -4.177019 0.000000

28 6 0 5.587318 -0.481478 0.000000

29 1 0 4.191372 -3.123531 0.000000

30 6 0 -5.587318 0.481478 0.000000

31 1 0 -4.191372 3.123531 0.000000

32 6 0 0.477569 5.572027 0.000000

33 1 0 3.129109 4.177019 0.000000

34 1 0 -1.330127 -6.253744 0.000000

35 1 0 0.138383 -5.792840 0.878617

36 1 0 0.138383 -5.792840 -0.878617

37 1 0 5.795482 0.137805 0.878545

38 1 0 5.795482 0.137805 -0.878545

39 1 0 6.276058 -1.327801 0.000000

40 1 0 -5.795482 -0.137805 0.878545

41 1 0 -5.795482 -0.137805 -0.878545

42 1 0 -6.276058 1.327801 0.000000

43 1 0 -0.138383 5.792840 0.878617

44 1 0 -0.138383 5.792840 -0.878617

45 1 0 1.330127 6.253744 0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.367194 0.000000

3 C 2.220978 1.353535 0.000000

4 C 2.274810 2.290116 1.468511 0.000000

5 C 1.445137 2.281097 2.275134 1.374773 0.000000

6 N 3.546721 2.436286 1.362909 2.501452 3.583888

7 C 4.258971 2.936251 2.377650 3.733850 4.644423

8 N 4.196711 2.842312 2.930706 4.398985 4.979269

9 C 5.534613 4.192983 4.253935 5.715076 6.343064

10 C 6.376069 5.010351 4.664609 6.025036 6.915726

11 C 5.733713 4.416952 3.754939 4.982311 6.027327

12 N 1.363716 2.436462 3.540173 3.589379 2.495452

13 C 3.763876 4.423825 5.729064 6.036378 4.977303

14 C 4.651998 4.985971 6.338510 6.900074 5.997304

15 C 4.265035 4.190538 5.516871 6.348670 5.704250

16 N 2.944655 2.838568 4.177807 4.984998 4.389766

17 C 2.375858 2.923759 4.235613 4.640308 3.717792

18 N 5.345608 5.007204 6.249557 7.267420 6.788983

19 N 4.947702 4.025146 4.927134 6.246778 6.239019

20 C 5.596708 4.927134 6.001301 7.212299 6.989952

21 C 7.017071 6.246778 7.212299 8.504819 8.384738

22 C 7.224093 6.239019 6.989952 8.384738 8.488564

23 C 6.041204 4.947702 5.596708 7.017071 7.224093

24 N 6.273864 5.013739 5.333667 6.801128 7.264544

25 Zn 3.020602 2.012573 3.000651 4.252409 4.244282

26 C 3.739664 3.714411 2.613649 1.488627 2.590640

27 H 2.245948 3.315665 3.334061 2.207328 1.081120

28 C 7.853970 6.487111 6.137613 7.472461 8.396144

29 H 6.338258 5.098449 4.202649 5.215564 6.406719

30 C 4.411702 5.377563 6.575515 6.574814 5.332214

31 H 5.720372 6.062575 7.415770 7.975711 7.044850

32 C 8.173989 7.540236 8.586487 9.823496 9.584757

33 H 8.226871 7.182261 7.833866 9.261279 9.451807

34 H 4.129870 4.424329 3.510958 2.141735 2.760211

35 H 4.318509 4.119285 2.930910 2.142659 3.299073

36 H 4.318509 4.119285 2.930910 2.142659 3.299073

37 H 8.257946 6.901921 6.657269 8.018206 8.879008

38 H 8.257946 6.901921 6.657269 8.018206 8.879008

39 H 8.398739 7.046735 6.504333 7.731947 8.779084

40 H 4.337200 5.405671 6.515019 6.374263 5.093914

41 H 4.337200 5.405671 6.515019 6.374263 5.093914

42 H 5.478428 6.383443 7.616126 7.660736 6.423353

43 H 8.264065 7.734896 8.838201 10.013551 9.687115

44 H 8.264065 7.734896 8.838201 10.013551 9.687115

45 H 9.107653 8.383515 9.350834 10.645940 10.496009

6 7 8 9 10

6 N 0.000000

7 C 1.324051 0.000000

8 N 2.413897 1.364794 0.000000

9 C 3.519311 2.232457 1.364595 0.000000

10 C 3.560016 2.294922 2.319619 1.500185 0.000000

11 C 2.482596 1.480722 2.300727 2.283106 1.352056

12 N 4.816668 5.355936 5.016892 6.266096 7.305953

13 C 6.841484 7.027628 6.263195 7.235396 8.552536

14 C 7.280925 7.221995 6.245833 7.006031 8.426942

15 C 6.263773 6.013531 4.924827 5.579067 7.027628

16 N 5.011495 4.924827 4.008816 4.919528 6.263195

17 C 5.343192 5.579067 4.919528 6.004760 7.235396

18 N 6.768557 6.263773 5.011495 5.343192 6.841484

19 N 5.007204 4.190538 2.838568 2.923759 4.423825

20 C 6.249557 5.516871 4.177807 4.235613 5.729064

21 C 7.267420 6.348670 4.984998 4.640308 6.036378

22 C 6.788983 5.704250 4.389766 3.717792 4.977303

23 C 5.345608 4.265035 2.944655 2.375858 3.763876

24 N 4.762290 3.516852 2.416427 1.318191 2.483749

25 Zn 3.384278 3.006766 2.004408 3.002380 4.276268

26 C 3.071099 4.394411 5.364165 6.572386 6.567227

27 H 4.605495 5.710556 6.056713 7.421028 7.989305

28 C 4.983382 3.760863 3.735564 2.630037 1.485421

29 H 2.841904 2.270535 3.330230 3.345426 2.188657

30 C 7.808487 8.175394 7.548559 8.602986 9.862370

31 H 8.335368 8.220343 7.182824 7.841224 9.296817

32 C 8.719297 7.830807 6.466231 6.114199 7.483019

33 H 7.494912 6.320478 5.082238 4.175468 5.217429

34 H 4.135730 5.459397 6.366748 7.610742 7.653224

35 H 3.077513 4.334046 5.406056 6.524699 6.375549

36 H 3.077513 4.334046 5.406056 6.524699 6.375549

37 H 5.571778 4.327960 4.126770 2.931095 2.134413

38 H 5.571778 4.327960 4.126770 2.931095 2.134413

39 H 5.236785 4.163860 4.453403 3.534017 2.139623

40 H 7.785811 8.252692 7.730586 8.842745 10.038631

41 H 7.785811 8.252692 7.730586 8.842745 10.038631

42 H 8.819675 9.113038 8.396810 9.372471 10.691065

43 H 9.062660 8.245820 6.892465 6.644779 8.038752

44 H 9.062660 8.245820 6.892465 6.644779 8.038752

45 H 9.357324 8.368594 7.018328 6.470107 7.730343

11 12 13 14 15

11 C 0.000000

12 N 6.834172 0.000000

13 C 8.426942 2.483749 0.000000

14 C 8.516862 3.540563 1.352056 0.000000

15 C 7.221995 3.516852 2.294922 1.480722 0.000000

16 N 6.245833 2.416427 2.319619 2.300727 1.364794

17 C 7.006031 1.318191 1.500185 2.283106 2.232457

18 N 7.280925 4.762290 3.560016 2.482596 1.324051

19 N 4.985971 5.013739 5.010351 4.416952 2.936251

20 C 6.338510 5.333667 4.664609 3.754939 2.377650

21 C 6.900074 6.801128 6.025036 4.982311 3.733850

22 C 5.997304 7.264544 6.915726 6.027327 4.644423

23 C 4.651998 6.273864 6.376069 5.733713 4.258971

24 N 3.540563 6.778351 7.305953 6.834172 5.355936

25 Zn 4.258431 3.389175 4.276268 4.258431 3.006766

26 C 5.344227 5.011197 7.483019 8.382053 7.830807

27 H 7.071349 2.860907 5.217429 6.382954 6.320478

28 C 2.575005 8.750409 9.862370 9.619652 8.175394

29 H 1.081389 7.534562 9.296817 9.473498 8.220343

30 C 9.619652 3.050124 1.485421 2.575005 3.760863

31 H 9.473498 4.566343 2.188657 1.081389 2.270535

32 C 8.382053 7.772518 6.567227 5.344227 4.394411

33 H 6.382954 8.322610 7.989305 7.071349 5.710556

34 H 6.435762 5.253118 7.730343 8.752516 8.368594

35 H 5.115208 5.608110 8.038752 8.876899 8.245820

36 H 5.115208 5.608110 8.038752 8.876899 8.245820

37 H 3.277570 9.079016 10.038631 9.709938 8.252692

38 H 3.277570 9.079016 10.038631 9.709938 8.252692

39 H 2.756822 9.399260 10.691065 10.534340 9.113038

40 H 9.709938 3.049817 2.134413 3.277570 4.327960

41 H 9.709938 3.049817 2.134413 3.277570 4.327960

42 H 10.534340 4.114711 2.139623 2.756822 4.163860

43 H 8.876899 7.760048 6.375549 5.115208 4.334046

44 H 8.876899 7.760048 6.375549 5.115208 4.334046

45 H 8.752516 8.782647 7.653224 6.435762 5.459397

16 17 18 19 20

16 N 0.000000

17 C 1.364595 0.000000

18 N 2.413897 3.519311 0.000000

19 N 2.842312 4.192983 2.436286 0.000000

20 C 2.930706 4.253935 1.362909 1.353535 0.000000

21 C 4.398985 5.715076 2.501452 2.290116 1.468511

22 C 4.979269 6.343064 3.583888 2.281097 2.275134

23 C 4.196711 5.534613 3.546721 1.367194 2.220978

24 N 5.016892 6.266096 4.816668 2.436462 3.540173

25 Zn 2.004408 3.002380 3.384278 2.012573 3.000651

26 C 6.466231 6.114199 8.719297 7.540236 8.586487

27 H 5.082238 4.175468 7.494912 7.182261 7.833866

28 C 7.548559 8.602986 7.808487 5.377563 6.575515

29 H 7.182824 7.841224 8.335368 6.062575 7.415770

30 C 3.735564 2.630037 4.983382 6.487111 6.137613

31 H 3.330230 3.345426 2.841904 5.098449 4.202649

32 C 5.364165 6.572386 3.071099 3.714411 2.613649

33 H 6.056713 7.421028 4.605495 3.315665 3.334061

34 H 7.018328 6.470107 9.357324 8.383515 9.350834

35 H 6.892465 6.644779 9.062660 7.734896 8.838201

36 H 6.892465 6.644779 9.062660 7.734896 8.838201

37 H 7.730586 8.842745 7.785811 5.405671 6.515019

38 H 7.730586 8.842745 7.785811 5.405671 6.515019

39 H 8.396810 9.372471 8.819675 6.383443 7.616126

40 H 4.126770 2.931095 5.571778 6.901921 6.657269

41 H 4.126770 2.931095 5.571778 6.901921 6.657269

42 H 4.453403 3.534017 5.236785 7.046735 6.504333

43 H 5.406056 6.524699 3.077513 4.119285 2.930910

44 H 5.406056 6.524699 3.077513 4.119285 2.930910

45 H 6.366748 7.610742 4.135730 4.424329 3.510958

21 22 23 24 25

21 C 0.000000

22 C 1.374773 0.000000

23 C 2.274810 1.445137 0.000000

24 N 3.589379 2.495452 1.363716 0.000000

25 Zn 4.252409 4.244282 3.020602 3.389175 0.000000

26 C 9.823496 9.584757 8.173989 7.772518 5.592455

27 H 9.261279 9.451807 8.226871 8.322610 5.219081

28 C 6.574814 5.332214 4.411702 3.050124 5.608025

29 H 7.975711 7.044850 5.720372 4.566343 5.227241

30 C 7.472461 8.396144 7.853970 8.750409 5.608025

31 H 5.215564 6.406719 6.338258 7.534562 5.227241

32 C 1.488627 2.590640 3.739664 5.011197 5.592455

33 H 2.207328 1.081120 2.245948 2.860907 5.219081

34 H 10.645940 10.496009 9.107653 8.782647 6.393634

35 H 10.013551 9.687115 8.264065 7.760048 5.860726

36 H 10.013551 9.687115 8.264065 7.760048 5.860726

37 H 6.374263 5.093914 4.337200 3.049817 5.863313

38 H 6.374263 5.093914 4.337200 3.049817 5.863313

39 H 7.660736 6.423353 5.478428 4.114711 6.414979

40 H 8.018206 8.879008 8.257946 9.079016 5.863313

41 H 8.018206 8.879008 8.257946 9.079016 5.863313

42 H 7.731947 8.779084 8.398739 9.399260 6.414979

43 H 2.142659 3.299073 4.318509 5.608110 5.860726

44 H 2.142659 3.299073 4.318509 5.608110 5.860726

45 H 2.141735 2.760211 4.129870 5.253118 6.393634

26 27 28 29 30

26 C 0.000000

27 H 2.996115 0.000000

28 C 7.918115 9.467477 0.000000

29 H 5.272015 7.395896 2.988162 0.000000

30 C 7.921771 5.267294 11.216050 10.422038 0.000000

31 H 9.455425 7.377427 10.422038 10.454482 2.988162

32 C 11.184911 10.394807 7.921771 9.455425 7.918115

33 H 10.394807 10.438162 5.267294 7.377427 9.467477

34 H 1.091601 2.747566 9.009445 6.347061 7.967866

35 H 1.095501 3.749579 7.659858 4.931926 8.539478

36 H 1.095501 3.749579 7.659858 4.931926 8.539478

37 H 8.527907 9.951777 1.094845 3.739161 11.421825

38 H 8.527907 9.951777 1.094845 3.739161 11.421825

39 H 7.976524 9.827268 1.091158 2.751465 12.000549

40 H 7.653940 4.919007 11.421825 10.460576 1.094845

41 H 7.653940 4.919007 11.421825 10.460576 1.094845

42 H 9.012774 6.340846 12.000549 11.374596 1.091158

43 H 11.403824 10.445788 8.539478 9.950900 7.659858

44 H 11.403824 10.445788 8.539478 9.950900 7.659858

45 H 11.963136 11.343967 7.967866 9.804082 9.009445

31 32 33 34 35

31 H 0.000000

32 C 5.272015 0.000000

33 H 7.395896 2.996115 0.000000

34 H 9.804082 11.963136 11.343967 0.000000

35 H 9.950900 11.403824 10.445788 1.772265 0.000000

36 H 9.950900 11.403824 10.445788 1.772265 1.757234

37 H 10.460576 7.653940 4.919007 9.612391 8.196055

38 H 10.460576 7.653940 4.919007 9.612391 8.382299

39 H 11.374596 9.012774 6.340846 9.061951 7.640654

40 H 3.739161 8.527907 9.951777 7.623381 8.196961

41 H 3.739161 8.527907 9.951777 7.623381 8.383185

42 H 2.751465 7.976524 9.827268 9.052185 9.623957

43 H 4.931926 1.095501 3.749579 12.137232 11.588984

44 H 4.931926 1.095501 3.749579 12.137232 11.721452

45 H 6.347061 1.091601 2.747566 12.787267 12.137232

36 37 38 39 40

36 H 0.000000

37 H 8.382299 0.000000

38 H 8.196055 1.757091 0.000000

39 H 7.640654 1.775048 1.775048 0.000000

40 H 8.383185 11.594240 11.726627 12.161826 0.000000

41 H 8.196961 11.726627 11.594240 12.161826 1.757091

42 H 9.623957 12.161826 12.161826 12.829958 1.775048

43 H 11.721452 8.196961 8.383185 9.623957 8.196055

44 H 11.588984 8.383185 8.196961 9.623957 8.382299

45 H 12.137232 7.623381 7.623381 9.052185 9.612391

41 42 43 44 45

41 H 0.000000

42 H 1.775048 0.000000

43 H 8.382299 7.640654 0.000000

44 H 8.196055 7.640654 1.757234 0.000000

45 H 9.612391 9.061951 1.772265 1.772265 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=0 Diff= 1.28D-03

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 2.807193 -1.115216 0.000000

2 7 0 2.012571 -0.002653 0.000000

3 6 0 2.789507 1.105692 0.000000

4 6 0 4.196731 0.685880 0.000000

5 6 0 4.188006 -0.688865 0.000000

6 7 0 2.380304 2.405721 0.000000

7 6 0 1.114082 2.792752 0.000000

8 7 0 0.000000 2.004408 0.000000

9 6 0 -1.118367 2.786313 0.000000

10 6 0 -0.681790 4.221568 0.000000

11 6 0 0.670170 4.205366 0.000000

12 7 0 2.381984 -2.410947 0.000000

13 6 0 0.681790 -4.221568 0.000000

14 6 0 -0.670170 -4.205366 0.000000

15 6 0 -1.114082 -2.792752 0.000000

16 7 0 -0.000000 -2.004408 0.000000

17 6 0 1.118367 -2.786313 0.000000

18 7 0 -2.380304 -2.405721 0.000000

19 7 0 -2.012571 0.002653 0.000000

20 6 0 -2.789507 -1.105692 0.000000

21 6 0 -4.196731 -0.685880 0.000000

22 6 0 -4.188006 0.688865 0.000000

23 6 0 -2.807193 1.115216 0.000000

24 7 0 -2.381984 2.410947 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 5.350812 1.626150 0.000000

27 1 0 5.040428 -1.353844 0.000000

28 6 0 -1.628201 5.366461 0.000000

29 1 0 1.343335 5.051683 0.000000

30 6 0 1.628201 -5.366461 0.000000

31 1 0 -1.343335 -5.051683 0.000000

32 6 0 -5.350812 -1.626150 0.000000

33 1 0 -5.040428 1.353844 0.000000

34 1 0 6.300419 1.087783 0.000000

35 1 0 5.327053 2.280055 0.878617

36 1 0 5.327053 2.280055 -0.878617

37 1 0 -2.280500 5.329721 0.878545

38 1 0 -2.280500 5.329721 -0.878545

39 1 0 -1.098230 6.320273 0.000000

40 1 0 2.280500 -5.329721 0.878545

41 1 0 2.280500 -5.329721 -0.878545

42 1 0 1.098230 -6.320273 0.000000

43 1 0 -5.327053 -2.280055 0.878617

44 1 0 -5.327053 -2.280055 -0.878617

45 1 0 -6.300419 -1.087783 0.000000

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

Rotational constants (GHZ): 0.1830554 0.1817619 0.0914085

Leave Link 202 at Tue Sep 17 14:21:25 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 101 beta electrons

nuclear repulsion energy 2761.6319155532 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= -0.1142277442 Hartrees.

Nuclear repulsion after empirical dispersion term = 2761.5176878090 Hartrees.

No density basis found on file 724.

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Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 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 = 3496

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.59D-10

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 140

GePol: Fraction of low-weight points (<1% of avg) = 4.00%

GePol: Cavity surface area = 382.144 Ang\*\*2

GePol: Cavity volume = 379.389 Ang\*\*3

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

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

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PCM non-electrostatic energy = -0.0107482804 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2761.5069395286 Hartrees.

Leave Link 301 at Tue Sep 17 14:21:25 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= 15327 LenP2D= 41262.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.85D-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 14:21:26 2019, MaxMem= 2415919104 cpu: 12.4

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:21:26 2019, MaxMem= 2415919104 cpu: 1.4

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= -0.000000 -0.000000 -0.000000

Rot= 1.000000 0.000000 -0.000000 -0.000695 Ang= -0.08 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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(AG) (AG) (BU) (BU) (BG) (BG) (AG) (AG) (BU) (BU)

(AG) (BU) (BU) (AG) (AG) (AU) (BG) (BG) (AG) (BU)

(AU) (BU) (AG) (AU) (BG) (BG) (AG) (AU) (AG) (BU)

(BU) (AU) (AG) (BU) (BU) (AG) (AG) (BG) (BU) (BU)

(BG) (AG) (BU) (BU) (AU) (AG) (BG) (AG) (AU) (AU)

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Virtual (AG) (AG) (AG) (AG) (AG) (AG) (AG) (AG) (AG) (AG)

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The electronic state of the initial guess is 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0183 S= 1.0061

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= -1276.14906784053

Leave Link 401 at Tue Sep 17 14:21:28 2019, MaxMem= 2415919104 cpu: 38.1

(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= 36666048.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.66D-15 for 3490.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.18D-15 for 3495 2629.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.66D-15 for 3490.

Iteration 1 A^-1\*A deviation from orthogonality is 8.33D-09 for 1983 1969.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.66D-15 for 654.

Iteration 2 A\*A^-1 deviation from orthogonality is 2.66D-15 for 2505 241.

Iteration 2 A^-1\*A deviation from unit magnitude is 8.88D-16 for 141.

Iteration 2 A^-1\*A deviation from orthogonality is 3.30D-16 for 1796 1408.

E= -1275.84230524140

DIIS: error= 5.00D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.84230524140 IErMin= 1 ErrMin= 5.00D-04

ErrMax= 5.00D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.71D-04 BMatP= 6.71D-04

IDIUse=3 WtCom= 9.95D-01 WtEn= 5.00D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.302 Goal= None Shift= 0.000

Gap= 0.393 Goal= None Shift= 0.000

RMSDP=4.77D-05 MaxDP=1.22D-03 OVMax= 7.04D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.77D-05 CP: 1.00D+00

E= -1275.84252693807 Delta-E= -0.000221696674 Rises=F Damp=F

DIIS: error= 2.20D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84252693807 IErMin= 2 ErrMin= 2.20D-04

ErrMax= 2.20D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.49D-05 BMatP= 6.71D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.20D-03

Coeff-Com: 0.125D+00 0.875D+00

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

Coeff: 0.125D+00 0.875D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.44D-05 MaxDP=7.82D-04 DE=-2.22D-04 OVMax= 4.18D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.44D-05 CP: 1.00D+00 1.02D+00

E= -1275.84251954652 Delta-E= 0.000007391546 Rises=F Damp=F

DIIS: error= 3.45D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1275.84252693807 IErMin= 2 ErrMin= 2.20D-04

ErrMax= 3.45D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.26D-04 BMatP= 7.49D-05

IDIUse=3 WtCom= 3.50D-01 WtEn= 6.50D-01

Coeff-Com: -0.149D-01 0.573D+00 0.442D+00

Coeff-En: 0.000D+00 0.575D+00 0.425D+00

Coeff: -0.522D-02 0.574D+00 0.431D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=8.58D-06 MaxDP=4.34D-04 DE= 7.39D-06 OVMax= 1.66D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 5.50D-06 CP: 1.00D+00 1.05D+00 5.54D-01

E= -1275.84254758492 Delta-E= -0.000028038394 Rises=F Damp=F

DIIS: error= 6.07D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84254758492 IErMin= 4 ErrMin= 6.07D-05

ErrMax= 6.07D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.85D-06 BMatP= 7.49D-05

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

Coeff-Com: -0.123D-01 0.186D+00 0.192D+00 0.634D+00

Coeff: -0.123D-01 0.186D+00 0.192D+00 0.634D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.11D-06 MaxDP=1.82D-04 DE=-2.80D-05 OVMax= 2.06D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.57D-06 CP: 1.00D+00 1.06D+00 6.18D-01 1.24D+00

E= -1275.84254915174 Delta-E= -0.000001566826 Rises=F Damp=F

DIIS: error= 4.52D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84254915174 IErMin= 5 ErrMin= 4.52D-05

ErrMax= 4.52D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.03D-06 BMatP= 2.85D-06

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

Coeff-Com: -0.453D-02 0.329D-01 0.579D-01 0.385D+00 0.529D+00

Coeff: -0.453D-02 0.329D-01 0.579D-01 0.385D+00 0.529D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.03D-06 MaxDP=9.14D-05 DE=-1.57D-06 OVMax= 1.41D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 9.48D-07 CP: 1.00D+00 1.07D+00 6.70D-01 1.51D+00 1.24D+00

E= -1275.84255002746 Delta-E= -0.000000875717 Rises=F Damp=F

DIIS: error= 4.30D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84255002746 IErMin= 6 ErrMin= 4.30D-05

ErrMax= 4.30D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.78D-07 BMatP= 1.03D-06

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

Coeff-Com: 0.367D-02-0.610D-01-0.501D-01-0.493D-01 0.758D-01 0.108D+01

Coeff: 0.367D-02-0.610D-01-0.501D-01-0.493D-01 0.758D-01 0.108D+01

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.61D-06 MaxDP=1.84D-04 DE=-8.76D-07 OVMax= 2.74D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 7.61D-07 CP: 1.00D+00 1.08D+00 7.57D-01 1.97D+00 1.96D+00

CP: 1.90D+00

E= -1275.84255108061 Delta-E= -0.000001053151 Rises=F Damp=F

DIIS: error= 3.07D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84255108061 IErMin= 7 ErrMin= 3.07D-05

ErrMax= 3.07D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.56D-07 BMatP= 2.78D-07

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

Coeff-Com: 0.508D-02-0.589D-01-0.700D-01-0.257D+00-0.433D+00 0.773D+00

Coeff-Com: 0.104D+01

Coeff: 0.508D-02-0.589D-01-0.700D-01-0.257D+00-0.433D+00 0.773D+00

Coeff: 0.104D+01

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.58D-06 MaxDP=2.26D-04 DE=-1.05D-06 OVMax= 3.47D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 6.44D-07 CP: 1.00D+00 1.10D+00 8.56D-01 2.55D+00 2.85D+00

CP: 3.00D+00 1.89D+00

E= -1275.84255200962 Delta-E= -0.000000929005 Rises=F Damp=F

DIIS: error= 2.05D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84255200962 IErMin= 8 ErrMin= 2.05D-05

ErrMax= 2.05D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.26D-08 BMatP= 2.56D-07

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

Coeff-Com: 0.622D-03 0.103D-01-0.370D-02-0.762D-01-0.330D+00-0.147D+00

Coeff-Com: 0.489D+00 0.106D+01

Coeff: 0.622D-03 0.103D-01-0.370D-02-0.762D-01-0.330D+00-0.147D+00

Coeff: 0.489D+00 0.106D+01

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.77D-06 MaxDP=1.94D-04 DE=-9.29D-07 OVMax= 2.92D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.82D-06 CP: 1.00D+00 1.11D+00 9.34D-01 3.00D+00 3.00D+00

CP: 3.00D+00 2.97D+00 2.49D+00

E= -1275.84255240875 Delta-E= -0.000000399136 Rises=F Damp=F

DIIS: error= 1.15D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84255240875 IErMin= 9 ErrMin= 1.15D-05

ErrMax= 1.15D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.17D-08 BMatP= 8.26D-08

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

Coeff-Com: -0.165D-02 0.309D-01 0.258D-01 0.545D-01-0.746D-01-0.362D+00

Coeff-Com: -0.950D-01 0.712D+00 0.710D+00

Coeff: -0.165D-02 0.309D-01 0.258D-01 0.545D-01-0.746D-01-0.362D+00

Coeff: -0.950D-01 0.712D+00 0.710D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.75D-06 MaxDP=8.61D-05 DE=-3.99D-07 OVMax= 1.34D-03

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.25D-06 CP: 1.00D+00 1.12D+00 9.70D-01 3.00D+00 3.00D+00

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

E= -1275.84255250412 Delta-E= -0.000000095370 Rises=F Damp=F

DIIS: error= 5.20D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84255250412 IErMin=10 ErrMin= 5.20D-06

ErrMax= 5.20D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.14D-08 BMatP= 5.17D-08

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

Coeff-Com: -0.112D-02 0.140D-01 0.167D-01 0.658D-01 0.778D-01-0.129D+00

Coeff-Com: -0.248D+00 0.184D-01 0.382D+00 0.803D+00

Coeff: -0.112D-02 0.140D-01 0.167D-01 0.658D-01 0.778D-01-0.129D+00

Coeff: -0.248D+00 0.184D-01 0.382D+00 0.803D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=6.89D-07 MaxDP=3.87D-05 DE=-9.54D-08 OVMax= 5.36D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 2.56D-07 CP: 1.00D+00 1.12D+00 9.83D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.72D+00 1.37D+00

E= -1275.84255252533 Delta-E= -0.000000021207 Rises=F Damp=F

DIIS: error= 2.70D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84255252533 IErMin=11 ErrMin= 2.70D-06

ErrMax= 2.70D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.71D-09 BMatP= 1.14D-08

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

Coeff-Com: -0.842D-04-0.262D-02 0.311D-03 0.183D-01 0.577D-01 0.544D-01

Coeff-Com: -0.115D+00-0.209D+00-0.605D-01 0.460D+00 0.796D+00

Coeff: -0.842D-04-0.262D-02 0.311D-03 0.183D-01 0.577D-01 0.544D-01

Coeff: -0.115D+00-0.209D+00-0.605D-01 0.460D+00 0.796D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.84D-07 MaxDP=2.45D-05 DE=-2.12D-08 OVMax= 3.74D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 8.95D-08 CP: 1.00D+00 1.12D+00 9.92D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.86D+00 1.66D+00

CP: 1.45D+00

E= -1275.84255253280 Delta-E= -0.000000007471 Rises=F Damp=F

DIIS: error= 1.26D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84255253280 IErMin=12 ErrMin= 1.26D-06

ErrMax= 1.26D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.73D-10 BMatP= 4.71D-09

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

Coeff-Com: 0.162D-03-0.389D-02-0.319D-02-0.173D-02 0.116D-01 0.546D-01

Coeff-Com: -0.210D-01-0.955D-01-0.110D+00 0.126D+00 0.356D+00 0.687D+00

Coeff: 0.162D-03-0.389D-02-0.319D-02-0.173D-02 0.116D-01 0.546D-01

Coeff: -0.210D-01-0.955D-01-0.110D+00 0.126D+00 0.356D+00 0.687D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.46D-07 MaxDP=7.78D-06 DE=-7.47D-09 OVMax= 1.13D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 3.76D-08 CP: 1.00D+00 1.12D+00 9.95D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.91D+00 1.74D+00

CP: 1.60D+00 1.14D+00

E= -1275.84255253399 Delta-E= -0.000000001193 Rises=F Damp=F

DIIS: error= 7.48D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84255253399 IErMin=13 ErrMin= 7.48D-07

ErrMax= 7.48D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.24D-10 BMatP= 9.73D-10

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

Coeff-Com: 0.133D-03-0.116D-02-0.219D-02-0.767D-02-0.182D-01 0.982D-02

Coeff-Com: 0.290D-01 0.376D-01-0.529D-01-0.108D+00-0.185D+00 0.461D+00

Coeff-Com: 0.837D+00

Coeff: 0.133D-03-0.116D-02-0.219D-02-0.767D-02-0.182D-01 0.982D-02

Coeff: 0.290D-01 0.376D-01-0.529D-01-0.108D+00-0.185D+00 0.461D+00

Coeff: 0.837D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.63D-07 MaxDP=8.26D-06 DE=-1.19D-09 OVMax= 1.26D-04

Cycle 14 Pass 1 IDiag 1:

RMSU= 2.47D-08 CP: 1.00D+00 1.12D+00 9.98D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.95D+00 1.84D+00

CP: 1.71D+00 1.47D+00 1.36D+00

E= -1275.84255253470 Delta-E= -0.000000000705 Rises=F Damp=F

DIIS: error= 2.58D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84255253470 IErMin=14 ErrMin= 2.58D-07

ErrMax= 2.58D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.90D-11 BMatP= 5.24D-10

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

Coeff-Com: 0.824D-05 0.678D-03 0.550D-04-0.228D-02-0.107D-01-0.121D-01

Coeff-Com: 0.169D-01 0.428D-01 0.908D-02-0.735D-01-0.189D+00 0.120D-01

Coeff-Com: 0.330D+00 0.876D+00

Coeff: 0.824D-05 0.678D-03 0.550D-04-0.228D-02-0.107D-01-0.121D-01

Coeff: 0.169D-01 0.428D-01 0.908D-02-0.735D-01-0.189D+00 0.120D-01

Coeff: 0.330D+00 0.876D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=6.42D-08 MaxDP=3.41D-06 DE=-7.05D-10 OVMax= 4.92D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 9.62D-09 CP: 1.00D+00 1.12D+00 9.99D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.97D+00 1.87D+00

CP: 1.76D+00 1.57D+00 1.70D+00 1.37D+00

E= -1275.84255253477 Delta-E= -0.000000000071 Rises=F Damp=F

DIIS: error= 1.30D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.84255253477 IErMin=15 ErrMin= 1.30D-07

ErrMax= 1.30D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.96D-11 BMatP= 5.90D-11

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

Coeff-Com: -0.216D-04 0.583D-03 0.487D-03 0.242D-03-0.187D-02-0.892D-02

Coeff-Com: 0.356D-02 0.144D-01 0.174D-01-0.157D-01-0.595D-01-0.920D-01

Coeff-Com: -0.444D-02 0.481D+00 0.664D+00

Coeff: -0.216D-04 0.583D-03 0.487D-03 0.242D-03-0.187D-02-0.892D-02

Coeff: 0.356D-02 0.144D-01 0.174D-01-0.157D-01-0.595D-01-0.920D-01

Coeff: -0.444D-02 0.481D+00 0.664D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.32D-08 MaxDP=7.14D-07 DE=-7.14D-11 OVMax= 8.66D-06

Cycle 16 Pass 1 IDiag 1:

RMSU= 4.58D-09 CP: 1.00D+00 1.12D+00 9.99D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.97D+00 1.88D+00

CP: 1.77D+00 1.61D+00 1.80D+00 1.54D+00 1.01D+00

E= -1275.84255253480 Delta-E= -0.000000000033 Rises=F Damp=F

DIIS: error= 6.09D-08 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1275.84255253480 IErMin=16 ErrMin= 6.09D-08

ErrMax= 6.09D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.42D-12 BMatP= 1.96D-11

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

Coeff-Com: -0.114D-04 0.162D-03 0.219D-03 0.461D-03 0.103D-02-0.192D-02

Coeff-Com: -0.481D-03-0.995D-03 0.679D-02 0.330D-02 0.360D-02-0.448D-01

Coeff-Com: -0.508D-01 0.814D-01 0.307D+00 0.695D+00

Coeff: -0.114D-04 0.162D-03 0.219D-03 0.461D-03 0.103D-02-0.192D-02

Coeff: -0.481D-03-0.995D-03 0.679D-02 0.330D-02 0.360D-02-0.448D-01

Coeff: -0.508D-01 0.814D-01 0.307D+00 0.695D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=7.80D-09 MaxDP=3.28D-07 DE=-3.27D-11 OVMax= 5.51D-06

Error on total polarization charges = 0.06467

SCF Done: E(UB3LYP) = -1275.84255253 A.U. after 16 cycles

NFock= 16 Conv=0.78D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0180 S= 1.0060

<L.S>= 0.000000000000E+00

KE= 1.320815229418D+03 PE=-8.574972481068D+03 EE= 3.216807759587D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.74

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0180, after 2.0002

Leave Link 502 at Tue Sep 17 14:22:53 2019, MaxMem= 2415919104 cpu: 1486.2

(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= 15327 LenP2D= 41262.

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 = 246

Leave Link 701 at Tue Sep 17 14:22:56 2019, MaxMem= 2415919104 cpu: 68.7

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 14:22:56 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 14:23:06 2019, MaxMem= 2415919104 cpu: 178.3

(Enter /home/blab/g09/l716.exe)

Dipole = 2.73558953D-13 1.17239551D-13-4.44089210D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.001964782 -0.001278906 -0.000000000

2 7 0.000635046 0.001876336 -0.000000000

3 6 -0.001928139 0.000222234 -0.000000000

4 6 0.000574112 -0.001077829 -0.000000000

5 6 0.000481784 -0.000065283 0.000000000

6 7 0.003484301 0.000251448 -0.000000000

7 6 -0.001970856 -0.000994707 0.000000000

8 7 -0.001075660 0.000550259 -0.000000000

9 6 -0.001180820 0.002601184 -0.000000000

10 6 -0.000856725 -0.002574419 -0.000000000

11 6 0.002055615 0.000862894 0.000000000

12 7 -0.003013598 0.003296098 -0.000000000

13 6 0.000856725 0.002574419 0.000000000

14 6 -0.002055615 -0.000862894 -0.000000000

15 6 0.001970856 0.000994707 -0.000000000

16 7 0.001075660 -0.000550259 -0.000000000

17 6 0.001180820 -0.002601184 -0.000000000

18 7 -0.003484301 -0.000251448 -0.000000000

19 7 -0.000635046 -0.001876336 -0.000000000

20 6 0.001928139 -0.000222234 -0.000000000

21 6 -0.000574112 0.001077829 -0.000000000

22 6 -0.000481784 0.000065283 0.000000000

23 6 -0.001964782 0.001278906 -0.000000000

24 7 0.003013598 -0.003296098 0.000000000

25 30 0.000000000 -0.000000000 0.000000000

26 6 -0.000632412 -0.000138318 0.000000000

27 1 0.000132903 -0.000211337 0.000000000

28 6 -0.000166329 -0.000612653 0.000000000

29 1 -0.000008029 0.000072402 0.000000000

30 6 0.000166329 0.000612653 0.000000000

31 1 0.000008029 -0.000072402 -0.000000000

32 6 0.000632412 0.000138318 0.000000000

33 1 -0.000132903 0.000211337 -0.000000000

34 1 0.000156025 -0.000035181 0.000000000

35 1 0.000057171 -0.000084076 -0.000385288

36 1 0.000057171 -0.000084076 0.000385288

37 1 0.000139951 0.000162513 -0.000318827

38 1 0.000139951 0.000162513 0.000318827

39 1 0.000003985 0.000159392 0.000000000

40 1 -0.000139951 -0.000162513 -0.000318827

41 1 -0.000139951 -0.000162513 0.000318827

42 1 -0.000003985 -0.000159392 0.000000000

43 1 -0.000057171 0.000084076 -0.000385288

44 1 -0.000057171 0.000084076 0.000385288

45 1 -0.000156025 0.000035181 -0.000000000

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

Cartesian Forces: Max 0.003484301 RMS 0.001057206

Leave Link 716 at Tue Sep 17 14:23:06 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 0.003246154 RMS 0.000507528

Search for a local minimum.

Step number 19 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 12 13 14 15

16 17 18 19

DE= -6.10D-04 DEPred=-6.35D-04 R= 9.61D-01

TightC=F SS= 1.41D+00 RLast= 5.07D-02 DXNew= 8.4090D-02 1.5217D-01

Trust test= 9.61D-01 RLast= 5.07D-02 DXMaxT set to 8.41D-02

ITU= 1 -1 -1 1 1 -1 1 1 1 -1 0 1 -1 1 1 1 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01312

Eigenvalues --- 0.01339 0.01341 0.01345 0.01346 0.01604

Eigenvalues --- 0.01623 0.01632 0.01640 0.01775 0.01792

Eigenvalues --- 0.01811 0.01822 0.01890 0.01908 0.01939

Eigenvalues --- 0.01949 0.01998 0.02000 0.02045 0.02048

Eigenvalues --- 0.02070 0.02088 0.02103 0.02111 0.02114

Eigenvalues --- 0.02205 0.02313 0.02317 0.02351 0.02373

Eigenvalues --- 0.04442 0.07213 0.07213 0.07224 0.07224

Eigenvalues --- 0.07321 0.07390 0.07401 0.08509 0.11834

Eigenvalues --- 0.14496 0.14499 0.15032 0.15765 0.15959

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16023 0.16198 0.16269 0.17572 0.19630

Eigenvalues --- 0.20740 0.22069 0.22098 0.23736 0.23843

Eigenvalues --- 0.23854 0.24469 0.24841 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25002

Eigenvalues --- 0.25139 0.28289 0.29896 0.30872 0.32470

Eigenvalues --- 0.33190 0.33199 0.33226 0.33282 0.33282

Eigenvalues --- 0.33543 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33724 0.33728 0.34391 0.34416

Eigenvalues --- 0.34437 0.34437 0.34671 0.35480 0.35543

Eigenvalues --- 0.35556 0.35561 0.35682 0.35682 0.35770

Eigenvalues --- 0.38098 0.38865 0.41641 0.41811 0.44024

Eigenvalues --- 0.46557 0.48347 0.48968 0.48986 0.50292

Eigenvalues --- 0.51356 0.51362 0.53046 0.54011 0.54016

Eigenvalues --- 0.54037 0.56325 0.56333 0.56852

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 1.47328 -0.47328

Cosine: 1.000 > 0.970

Length: 1.000

GDIIS step was calculated using 2 of the last 19 vectors.

Iteration 1 RMS(Cart)= 0.00482448 RMS(Int)= 0.00001176

Iteration 2 RMS(Cart)= 0.00002066 RMS(Int)= 0.00000352

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000352

ITry= 1 IFail=0 DXMaxC= 1.94D-02 DCOld= 1.00D+10 DXMaxT= 8.41D-02 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 2.41D-09 for atom 29.

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

(Linear) (Quad) (Total)

R1 2.58362 0.00017 0.00013 -0.00190 -0.00178 2.58184

R2 2.73091 0.00081 0.00222 0.00171 0.00393 2.73484

R3 2.57705 0.00325 0.00693 0.00583 0.01276 2.58981

R4 2.55781 0.00105 0.00226 0.00648 0.00874 2.56655

R5 3.80321 -0.00078 -0.00038 -0.00239 -0.00279 3.80042

R6 2.77508 0.00041 -0.00062 0.00178 0.00116 2.77624

R7 2.57553 0.00169 0.00166 0.00341 0.00507 2.58060

R8 2.59794 0.00004 -0.00058 -0.00138 -0.00195 2.59599

R9 2.81310 0.00022 0.00178 -0.00316 -0.00138 2.81172

R10 2.04302 -0.00001 -0.00048 0.00111 0.00063 2.04365

R11 2.50209 -0.00177 0.00041 -0.00568 -0.00527 2.49682

R12 2.57909 0.00092 0.00119 0.00392 0.00511 2.58420

R13 2.79816 0.00066 0.00016 0.00132 0.00147 2.79963

R14 2.57871 0.00009 0.00082 -0.00149 -0.00065 2.57806

R15 3.78778 -0.00054 0.00033 0.00102 0.00135 3.78913

R16 2.83494 0.00125 0.00186 0.00453 0.00639 2.84133

R17 2.49102 -0.00122 0.00129 -0.00707 -0.00577 2.48525

R18 2.55502 -0.00200 -0.00235 -0.00313 -0.00548 2.54954

R19 2.80704 0.00007 -0.00065 0.00044 -0.00021 2.80683

R20 2.04353 -0.00007 0.00078 -0.00303 -0.00224 2.04129

R21 2.49102 -0.00122 0.00129 -0.00707 -0.00577 2.48525

R22 2.55502 -0.00200 -0.00235 -0.00313 -0.00548 2.54954

R23 2.83494 0.00125 0.00186 0.00453 0.00639 2.84133

R24 2.80704 0.00007 -0.00065 0.00044 -0.00021 2.80683

R25 2.79816 0.00066 0.00016 0.00132 0.00147 2.79963

R26 2.04353 -0.00007 0.00078 -0.00303 -0.00224 2.04129

R27 2.57909 0.00092 0.00119 0.00392 0.00511 2.58420

R28 2.50209 -0.00177 0.00041 -0.00568 -0.00527 2.49682

R29 2.57871 0.00009 0.00082 -0.00149 -0.00065 2.57806

R30 3.78778 -0.00054 0.00033 0.00102 0.00135 3.78913

R31 2.57553 0.00169 0.00166 0.00341 0.00507 2.58060

R32 2.55781 0.00105 0.00226 0.00648 0.00874 2.56655

R33 2.58362 0.00017 0.00013 -0.00190 -0.00178 2.58184

R34 3.80321 -0.00078 -0.00038 -0.00239 -0.00279 3.80042

R35 2.77508 0.00041 -0.00062 0.00178 0.00116 2.77624

R36 2.59794 0.00004 -0.00058 -0.00138 -0.00195 2.59599

R37 2.81310 0.00022 0.00178 -0.00316 -0.00138 2.81172

R38 2.73091 0.00081 0.00222 0.00171 0.00393 2.73484

R39 2.04302 -0.00001 -0.00048 0.00111 0.00063 2.04365

R40 2.57705 0.00325 0.00693 0.00583 0.01276 2.58981

R41 2.06283 -0.00010 -0.00026 -0.00126 -0.00152 2.06131

R42 2.07020 -0.00026 -0.00032 -0.00227 -0.00259 2.06761

R43 2.07020 -0.00026 -0.00032 -0.00227 -0.00259 2.06761

R44 2.06896 -0.00014 -0.00024 -0.00147 -0.00171 2.06725

R45 2.06896 -0.00014 -0.00024 -0.00147 -0.00171 2.06725

R46 2.06199 -0.00012 -0.00043 -0.00069 -0.00112 2.06086

R47 2.06896 -0.00014 -0.00024 -0.00147 -0.00171 2.06725

R48 2.06896 -0.00014 -0.00024 -0.00147 -0.00171 2.06725

R49 2.06199 -0.00012 -0.00043 -0.00069 -0.00112 2.06086

R50 2.07020 -0.00026 -0.00032 -0.00227 -0.00259 2.06761

R51 2.07020 -0.00026 -0.00032 -0.00227 -0.00259 2.06761

R52 2.06283 -0.00010 -0.00026 -0.00126 -0.00152 2.06131

A1 1.89153 -0.00022 -0.00100 -0.00016 -0.00116 1.89036

A2 2.20429 -0.00016 0.00059 0.00358 0.00416 2.20845

A3 2.18737 0.00038 0.00042 -0.00342 -0.00300 2.18437

A4 1.90999 -0.00033 -0.00152 0.00230 0.00079 1.91078

A5 2.19232 -0.00009 -0.00176 -0.00025 -0.00201 2.19031

A6 2.18087 0.00042 0.00328 -0.00205 0.00123 2.18209

A7 1.89226 0.00050 0.00256 -0.00496 -0.00240 1.88986

A8 2.22526 -0.00014 -0.00144 0.00269 0.00124 2.22650

A9 2.16566 -0.00035 -0.00112 0.00227 0.00116 2.16682

A10 1.85437 -0.00060 -0.00231 0.00338 0.00107 1.85544

A11 2.16801 0.00088 0.00497 0.00007 0.00504 2.17305

A12 2.26080 -0.00028 -0.00265 -0.00345 -0.00611 2.25470

A13 1.87662 0.00066 0.00228 -0.00057 0.00171 1.87833

A14 2.17962 -0.00007 0.00110 0.00152 0.00262 2.18224

A15 2.22694 -0.00058 -0.00337 -0.00095 -0.00433 2.22262

A16 2.17238 -0.00088 -0.00188 -0.00352 -0.00540 2.16698

A17 2.22913 0.00055 0.00047 0.00280 0.00328 2.23241

A18 2.17191 -0.00088 -0.00268 0.00153 -0.00115 2.17076

A19 1.88214 0.00033 0.00221 -0.00433 -0.00213 1.88001

A20 1.91562 -0.00049 -0.00124 0.00309 0.00185 1.91747

A21 2.18662 0.00044 0.00215 -0.00049 0.00165 2.18827

A22 2.18095 0.00005 -0.00090 -0.00260 -0.00350 2.17745

A23 1.88566 -0.00040 -0.00151 -0.00175 -0.00326 1.88240

A24 2.24268 0.00056 0.00016 0.00803 0.00820 2.25088

A25 2.15484 -0.00016 0.00134 -0.00627 -0.00494 2.14990

A26 1.85410 0.00084 0.00277 -0.00063 0.00214 1.85624

A27 2.15553 -0.00020 0.00167 -0.00127 0.00040 2.15593

A28 2.27355 -0.00064 -0.00444 0.00191 -0.00253 2.27102

A29 1.88726 -0.00027 -0.00223 0.00363 0.00141 1.88866

A30 2.16518 0.00016 0.00157 -0.00225 -0.00068 2.16450

A31 2.23075 0.00011 0.00065 -0.00138 -0.00073 2.23002

A32 2.17664 -0.00075 -0.00067 -0.00818 -0.00885 2.16779

A33 1.85410 0.00084 0.00277 -0.00063 0.00214 1.85624

A34 2.27355 -0.00064 -0.00444 0.00191 -0.00253 2.27102

A35 2.15553 -0.00020 0.00167 -0.00127 0.00040 2.15593

A36 1.88726 -0.00027 -0.00223 0.00363 0.00141 1.88866

A37 2.23075 0.00011 0.00065 -0.00138 -0.00073 2.23002

A38 2.16518 0.00016 0.00157 -0.00225 -0.00068 2.16450

A39 1.88214 0.00033 0.00221 -0.00433 -0.00213 1.88001

A40 2.17191 -0.00088 -0.00268 0.00153 -0.00115 2.17076

A41 2.22913 0.00055 0.00047 0.00280 0.00328 2.23241

A42 1.91562 -0.00049 -0.00124 0.00309 0.00185 1.91747

A43 2.18662 0.00044 0.00215 -0.00049 0.00165 2.18827

A44 2.18095 0.00005 -0.00090 -0.00260 -0.00350 2.17745

A45 2.15484 -0.00016 0.00134 -0.00627 -0.00494 2.14990

A46 2.24268 0.00056 0.00016 0.00803 0.00820 2.25088

A47 1.88566 -0.00040 -0.00151 -0.00175 -0.00326 1.88240

A48 2.17238 -0.00088 -0.00188 -0.00352 -0.00540 2.16698

A49 1.90999 -0.00033 -0.00152 0.00230 0.00079 1.91078

A50 2.18087 0.00042 0.00328 -0.00205 0.00123 2.18209

A51 2.19232 -0.00009 -0.00176 -0.00025 -0.00201 2.19031

A52 2.22526 -0.00014 -0.00144 0.00269 0.00124 2.22650

A53 2.16566 -0.00035 -0.00112 0.00227 0.00116 2.16682

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A55 1.85437 -0.00060 -0.00231 0.00338 0.00107 1.85544

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A57 2.26080 -0.00028 -0.00265 -0.00345 -0.00611 2.25470

A58 1.87662 0.00066 0.00228 -0.00057 0.00171 1.87833

A59 2.22694 -0.00058 -0.00337 -0.00095 -0.00433 2.22262

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A61 1.89153 -0.00022 -0.00100 -0.00016 -0.00116 1.89036

A62 2.20429 -0.00016 0.00059 0.00358 0.00416 2.20845

A63 2.18737 0.00038 0.00042 -0.00342 -0.00300 2.18437

A64 2.17664 -0.00075 -0.00067 -0.00818 -0.00885 2.16779

A65 1.57211 -0.00039 -0.00258 0.00058 -0.00200 1.57011

A66 1.56948 0.00039 0.00258 -0.00058 0.00200 1.57148

A67 1.56948 0.00039 0.00258 -0.00058 0.00200 1.57148

A68 1.57211 -0.00039 -0.00258 0.00058 -0.00200 1.57011

A69 1.94218 0.00015 -0.00047 0.00208 0.00160 1.94378

A70 1.93929 0.00018 0.00190 0.00006 0.00195 1.94124

A71 1.93929 0.00018 0.00190 0.00006 0.00195 1.94124

A72 1.88941 -0.00010 0.00001 0.00037 0.00038 1.88979

A73 1.88941 -0.00010 0.00001 0.00037 0.00038 1.88979

A74 1.86135 -0.00036 -0.00355 -0.00313 -0.00668 1.85467

A75 1.93236 0.00024 0.00177 0.00096 0.00272 1.93508

A76 1.93236 0.00024 0.00177 0.00096 0.00272 1.93508

A77 1.94366 0.00011 -0.00081 0.00505 0.00422 1.94788

A78 1.86274 -0.00043 -0.00346 -0.00593 -0.00939 1.85335

A79 1.89516 -0.00010 0.00030 -0.00078 -0.00049 1.89467

A80 1.89516 -0.00010 0.00030 -0.00078 -0.00049 1.89467

A81 1.93236 0.00024 0.00177 0.00096 0.00272 1.93508

A82 1.93236 0.00024 0.00177 0.00096 0.00272 1.93508

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A86 1.89516 -0.00010 0.00030 -0.00078 -0.00049 1.89467

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A88 1.93929 0.00018 0.00190 0.00006 0.00195 1.94124

A89 1.94218 0.00015 -0.00047 0.00208 0.00160 1.94378

A90 1.86135 -0.00036 -0.00355 -0.00313 -0.00668 1.85467

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D18 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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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

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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 1.03475 -0.00011 -0.00099 -0.00193 -0.00292 1.03183

D31 -1.03475 0.00011 0.00099 0.00193 0.00292 -1.03183

D32 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.10684 -0.00011 -0.00099 -0.00193 -0.00292 -2.10976

D34 2.10684 0.00011 0.00099 0.00193 0.00292 2.10976

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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 1.03118 -0.00012 -0.00104 -0.00307 -0.00412 1.02706

D64 -1.03118 0.00012 0.00104 0.00307 0.00412 -1.02706

D65 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D66 -2.11041 -0.00012 -0.00104 -0.00307 -0.00412 -2.11453

D67 2.11041 0.00012 0.00104 0.00307 0.00412 2.11453

D68 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

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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 -2.11041 -0.00012 -0.00104 -0.00307 -0.00412 -2.11453

D80 2.11041 0.00012 0.00104 0.00307 0.00412 2.11453

D81 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

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D83 -1.03118 0.00012 0.00104 0.00307 0.00412 -1.02706

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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

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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

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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

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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 1.03475 -0.00011 -0.00099 -0.00193 -0.00292 1.03183

D126 -1.03475 0.00011 0.00099 0.00193 0.00292 -1.03183

D127 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D128 -2.10684 -0.00011 -0.00099 -0.00193 -0.00292 -2.10976

D129 2.10684 0.00011 0.00099 0.00193 0.00292 2.10976

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

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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 0.003246 0.000450 NO

RMS Force 0.000508 0.000300 NO

Maximum Displacement 0.019383 0.001800 NO

RMS Displacement 0.004822 0.001200 NO

Predicted change in Energy=-1.494124D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:23:07 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 -2.074008 -2.190995 0.000000

2 7 0 -0.746639 -1.867363 0.000000

3 6 0 -0.003318 -3.004055 0.000000

4 6 0 -0.918611 -4.153213 0.000000

5 6 0 -2.190262 -3.633534 0.000000

6 7 0 1.358274 -3.108518 0.000000

7 6 0 2.181613 -2.075152 0.000000

8 7 0 1.861306 -0.745692 0.000000

9 6 0 3.000131 0.005476 0.000000

10 6 0 4.172945 -0.935388 0.000000

11 6 0 3.659192 -2.182898 0.000000

12 7 0 -3.127487 -1.314432 0.000000

13 6 0 -4.172945 0.935388 0.000000

14 6 0 -3.659192 2.182898 0.000000

15 6 0 -2.181613 2.075152 0.000000

16 7 0 -1.861306 0.745692 0.000000

17 6 0 -3.000131 -0.005476 0.000000

18 7 0 -1.358274 3.108518 0.000000

19 7 0 0.746639 1.867363 0.000000

20 6 0 0.003318 3.004055 0.000000

21 6 0 0.918611 4.153213 0.000000

22 6 0 2.190262 3.633534 0.000000

23 6 0 2.074008 2.190995 0.000000

24 7 0 3.127487 1.314432 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.484669 -5.576425 0.000000

27 1 0 -3.122790 -4.181200 0.000000

28 6 0 5.587654 -0.482897 0.000000

29 1 0 4.196781 -3.119825 0.000000

30 6 0 -5.587654 0.482897 0.000000

31 1 0 -4.196781 3.119825 0.000000

32 6 0 0.484669 5.576425 0.000000

33 1 0 3.122790 4.181200 0.000000

34 1 0 -1.340384 -6.252882 0.000000

35 1 0 0.131566 -5.802645 0.875332

36 1 0 0.131566 -5.802645 -0.875332

37 1 0 5.797781 0.139499 0.874744

38 1 0 5.797781 0.139499 -0.874744

39 1 0 6.279015 -1.326310 0.000000

40 1 0 -5.797781 -0.139499 0.874744

41 1 0 -5.797781 -0.139499 -0.874744

42 1 0 -6.279015 1.326310 0.000000

43 1 0 -0.131566 5.802645 0.875332

44 1 0 -0.131566 5.802645 -0.875332

45 1 0 1.340384 6.252882 0.000000

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Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.366252 0.000000

3 C 2.224595 1.358159 0.000000

4 C 2.277112 2.292310 1.469124 0.000000

5 C 1.447215 2.281098 2.275735 1.373740 0.000000

6 N 3.552803 2.443589 1.365593 2.505114 3.587165

7 C 4.257197 2.935615 2.374191 3.732255 4.641320

8 N 4.192326 2.838930 2.928656 4.397629 4.975423

9 C 5.529138 4.188772 4.251821 5.714126 6.338972

10 C 6.371889 5.007084 4.660532 6.023151 6.911613

11 C 5.733206 4.417116 3.753436 4.983817 6.026646

12 N 1.370468 2.444212 3.551797 3.596917 2.501324

13 C 3.765609 4.426622 5.736288 6.040244 4.980570

14 C 4.652284 4.988745 6.345857 6.903411 5.999052

15 C 4.267504 4.195542 5.526600 6.355132 5.708692

16 N 2.944380 2.840869 4.184821 4.988782 4.391563

17 C 2.373647 2.923157 4.239383 4.640738 3.717350

18 N 5.347627 5.013331 6.260947 7.275028 6.793192

19 N 4.942299 4.022195 4.928808 6.246630 6.235804

20 C 5.594983 4.928808 6.008114 7.216401 6.990664

21 C 7.014610 6.246630 7.216401 8.507179 8.384421

22 C 7.218666 6.235804 6.990664 8.384421 8.485238

23 C 6.033894 4.942299 5.594983 7.014610 7.218666

24 N 6.272445 5.013250 5.333973 6.801915 7.263664

25 Zn 3.016947 2.011098 3.004057 4.253590 4.242619

26 C 3.739937 3.718302 2.617018 1.487897 2.585319

27 H 2.249635 3.316615 3.334183 2.204356 1.081455

28 C 7.849756 6.483827 6.133124 7.470121 8.391811

29 H 6.339205 5.099615 4.201694 5.218729 6.407669

30 C 4.415361 5.381370 6.583589 6.579777 5.337347

31 H 5.719352 6.064283 7.422065 7.977687 7.045138

32 C 8.177997 7.544938 8.594345 9.830312 9.590547

33 H 8.222626 7.180361 7.835843 9.262579 9.449793

34 H 4.127605 4.425529 3.513207 2.141612 2.753775

35 H 4.321432 4.126002 2.935388 2.142359 3.295775

36 H 4.321432 4.126002 2.935388 2.142359 3.295775

37 H 8.255995 6.900878 6.655814 8.018883 8.877488

38 H 8.255995 6.900878 6.655814 8.018883 8.877488

39 H 8.397659 7.046457 6.502502 7.732865 8.777923

40 H 4.340542 5.409688 6.522780 6.378195 5.097808

41 H 4.340542 5.409688 6.522780 6.378195 5.097808

42 H 5.482110 6.388015 7.624726 7.665449 6.427904

43 H 8.272700 7.744258 8.851024 10.025206 9.697726

44 H 8.272700 7.744258 8.851024 10.025206 9.697726

45 H 9.108081 8.384154 9.353952 10.648468 10.497936

6 7 8 9 10

6 N 0.000000

7 C 1.321262 0.000000

8 N 2.415779 1.367501 0.000000

9 C 3.520320 2.235840 1.364249 0.000000

10 C 3.555962 2.294442 2.319409 1.503569 0.000000

11 C 2.480120 1.481503 2.301728 2.285463 1.349156

12 N 4.831232 5.363324 5.021108 6.268162 7.310266

13 C 6.851829 7.031625 6.264042 7.233101 8.552993

14 C 7.292054 7.228139 6.249203 7.006265 8.430070

15 C 6.277040 6.021857 4.929742 5.579787 7.031625

16 N 5.022015 4.929742 4.010246 4.917468 6.264042

17 C 5.350193 5.579787 4.917468 6.000271 7.233101

18 N 6.784627 6.277040 5.022015 5.350193 6.851829

19 N 5.013331 4.195542 2.840869 2.923157 4.426622

20 C 6.260947 5.526600 4.184821 4.239383 5.736288

21 C 7.275028 6.355132 4.988782 4.640738 6.040244

22 C 6.793192 5.708692 4.391563 3.717350 4.980570

23 C 5.347627 4.267504 2.944380 2.373647 3.765609

24 N 4.763675 3.519084 2.418124 1.315137 2.480861

25 Zn 3.392314 3.010928 2.005123 3.000136 4.276496

26 C 3.080098 4.400906 5.370249 6.580383 6.575150

27 H 4.607665 5.707200 6.053423 7.417440 7.985176

28 C 4.978106 3.759839 3.735603 2.633208 1.485311

29 H 2.838530 2.269856 3.330308 3.346563 2.184567

30 C 7.819474 8.179555 7.549599 8.601045 9.863104

31 H 8.345712 8.226281 7.186282 7.841857 9.300380

32 C 8.728769 7.837489 6.470262 6.112530 7.483788

33 H 7.500233 6.326749 5.085824 4.177525 5.223246

34 H 4.143644 5.464238 6.370240 7.616240 7.659800

35 H 3.086963 4.343167 5.415808 6.536753 6.386638

36 H 3.086963 4.343167 5.415808 6.536753 6.386638

37 H 5.569921 4.329726 4.128508 2.934278 2.135569

38 H 5.569921 4.329726 4.128508 2.934278 2.135569

39 H 5.233541 4.165269 4.455701 3.539031 2.142044

40 H 7.796754 8.257279 7.732675 8.842480 10.040617

41 H 7.796754 8.257279 7.732675 8.842480 10.040617

42 H 8.831528 9.118781 8.399882 9.372681 10.693865

43 H 9.077150 8.256917 6.900613 6.646871 8.043389

44 H 9.077150 8.256917 6.900613 6.646871 8.043389

45 H 9.361416 8.370412 7.017934 6.464119 7.726229

11 12 13 14 15

11 C 0.000000

12 N 6.842021 0.000000

13 C 8.430070 2.480861 0.000000

14 C 8.521673 3.537516 1.349156 0.000000

15 C 7.228139 3.519084 2.294442 1.481503 0.000000

16 N 6.249203 2.418124 2.319409 2.301728 1.367501

17 C 7.006265 1.315137 1.503569 2.285463 2.235840

18 N 7.292054 4.763675 3.555962 2.480120 1.321262

19 N 4.988745 5.013250 5.007084 4.417116 2.935615

20 C 6.345857 5.333973 4.660532 3.753436 2.374191

21 C 6.903411 6.801915 6.023151 4.983817 3.732255

22 C 5.999052 7.263664 6.911613 6.026646 4.641320

23 C 4.652284 6.272445 6.371889 5.733206 4.257197

24 N 3.537516 6.784956 7.310266 6.842021 5.363324

25 Zn 4.260837 3.392478 4.276496 4.260837 3.010928

26 C 5.356082 5.014885 7.483788 8.383596 7.837489

27 H 7.070254 2.866772 5.223246 6.386663 6.326749

28 C 2.570791 8.754721 9.863104 9.623442 8.179555

29 H 1.080202 7.543498 9.300380 9.478143 8.226281

30 C 9.623442 3.046770 1.485311 2.570791 3.759839

31 H 9.478143 4.561362 2.184567 1.080202 2.269856

32 C 8.383596 7.780204 6.575150 5.356082 4.400906

33 H 6.386663 8.322736 7.985176 7.070254 5.707200

34 H 6.446746 5.251859 7.726229 8.748671 8.370412

35 H 5.129612 5.615308 8.043389 8.882845 8.256917

36 H 5.129612 5.615308 8.043389 8.882845 8.256917

37 H 3.276014 9.085126 10.040617 9.714680 8.257279

38 H 3.276014 9.085126 10.040617 9.714680 8.257279

39 H 2.756304 9.406510 10.693865 10.539569 9.118781

40 H 9.714680 3.045671 2.135569 3.276014 4.329726

41 H 9.714680 3.045671 2.135569 3.276014 4.329726

42 H 10.539569 4.111648 2.142044 2.756304 4.165269

43 H 8.882845 7.771392 6.386638 5.129612 4.343167

44 H 8.882845 7.771392 6.386638 5.129612 4.343167

45 H 8.748671 8.787839 7.659800 6.446746 5.464238

16 17 18 19 20

16 N 0.000000

17 C 1.364249 0.000000

18 N 2.415779 3.520320 0.000000

19 N 2.838930 4.188772 2.443589 0.000000

20 C 2.928656 4.251821 1.365593 1.358159 0.000000

21 C 4.397629 5.714126 2.505114 2.292310 1.469124

22 C 4.975423 6.338972 3.587165 2.281098 2.275735

23 C 4.192326 5.529138 3.552803 1.366252 2.224595

24 N 5.021108 6.268162 4.831232 2.444212 3.551797

25 Zn 2.005123 3.000136 3.392314 2.011098 3.004057

26 C 6.470262 6.112530 8.728769 7.544938 8.594345

27 H 5.085824 4.177525 7.500233 7.180361 7.835843

28 C 7.549599 8.601045 7.819474 5.381370 6.583589

29 H 7.186282 7.841857 8.345712 6.064283 7.422065

30 C 3.735603 2.633208 4.978106 6.483827 6.133124

31 H 3.330308 3.346563 2.838530 5.099615 4.201694

32 C 5.370249 6.580383 3.080098 3.718302 2.617018

33 H 6.053423 7.417440 4.607665 3.316615 3.334183

34 H 7.017934 6.464119 9.361416 8.384154 9.353952

35 H 6.900613 6.646871 9.077150 7.744258 8.851024

36 H 6.900613 6.646871 9.077150 7.744258 8.851024

37 H 7.732675 8.842480 7.796754 5.409688 6.522780

38 H 7.732675 8.842480 7.796754 5.409688 6.522780

39 H 8.399882 9.372681 8.831528 6.388015 7.624726

40 H 4.128508 2.934278 5.569921 6.900878 6.655814

41 H 4.128508 2.934278 5.569921 6.900878 6.655814

42 H 4.455701 3.539031 5.233541 7.046457 6.502502

43 H 5.415808 6.536753 3.086963 4.126002 2.935388

44 H 5.415808 6.536753 3.086963 4.126002 2.935388

45 H 6.370240 7.616240 4.143644 4.425529 3.513207

21 22 23 24 25

21 C 0.000000

22 C 1.373740 0.000000

23 C 2.277112 1.447215 0.000000

24 N 3.596917 2.501324 1.370468 0.000000

25 Zn 4.253590 4.242619 3.016947 3.392478 0.000000

26 C 9.830312 9.590547 8.177997 7.780204 5.597447

27 H 9.262579 9.449793 8.222626 8.322736 5.218644

28 C 6.579777 5.337347 4.415361 3.046770 5.608482

29 H 7.977687 7.045138 5.719352 4.561362 5.229367

30 C 7.470121 8.391811 7.849756 8.754721 5.608482

31 H 5.218729 6.407669 6.339205 7.543498 5.229367

32 C 1.487897 2.585319 3.739937 5.014885 5.597447

33 H 2.204356 1.081455 2.249635 2.866772 5.218644

34 H 10.648468 10.497936 9.108081 8.787839 6.394932

35 H 10.025206 9.697726 8.272700 7.771392 5.869770

36 H 10.025206 9.697726 8.272700 7.771392 5.869770

37 H 6.378195 5.097808 4.340542 3.045671 5.865058

38 H 6.378195 5.097808 4.340542 3.045671 5.865058

39 H 7.665449 6.427904 5.482110 4.111648 6.417564

40 H 8.018883 8.877488 8.255995 9.085126 5.865058

41 H 8.018883 8.877488 8.255995 9.085126 5.865058

42 H 7.732865 8.777923 8.397659 9.406510 6.417564

43 H 2.142359 3.295775 4.321432 5.615308 5.869770

44 H 2.142359 3.295775 4.321432 5.615308 5.869770

45 H 2.141612 2.753775 4.127605 5.251859 6.394932

26 27 28 29 30

26 C 0.000000

27 H 2.984348 0.000000

28 C 7.925726 9.463048 0.000000

29 H 5.286857 7.396123 2.981261 0.000000

30 C 7.921858 5.275354 11.216963 10.426638 0.000000

31 H 9.455397 7.379596 10.426638 10.458735 2.981261

32 C 11.194895 10.403124 7.921858 9.455397 7.925726

33 H 10.403124 10.437289 5.275354 7.379596 9.463048

34 H 1.090799 2.732916 9.016121 6.362094 7.963040

35 H 1.094133 3.739802 7.670386 4.948707 8.543051

36 H 1.094133 3.739802 7.670386 4.948707 8.543051

37 H 8.538510 9.950387 1.093942 3.735181 11.424151

38 H 8.538510 9.950387 1.093942 3.735181 11.424151

39 H 7.988172 9.825697 1.090563 2.748162 12.003794

40 H 7.652091 4.925048 11.424151 10.466079 1.093942

41 H 7.652091 4.925048 11.424151 10.466079 1.093942

42 H 9.012336 6.347789 12.003794 11.380265 1.090563

43 H 11.418148 10.459005 8.543051 9.955464 7.670386

44 H 11.418148 10.459005 8.543051 9.955464 7.670386

45 H 11.969265 11.348567 7.963040 9.798298 9.016121

31 32 33 34 35

31 H 0.000000

32 C 5.286857 0.000000

33 H 7.396123 2.984348 0.000000

34 H 9.798298 11.969265 11.348567 0.000000

35 H 9.955464 11.418148 10.459005 1.770750 0.000000

36 H 9.955464 11.418148 10.459005 1.770750 1.750664

37 H 10.466079 7.652091 4.925048 9.621908 8.210668

38 H 10.466079 7.652091 4.925048 9.621908 8.395108

39 H 11.380265 9.012336 6.347789 9.073387 7.654731

40 H 3.735181 8.538510 9.950387 7.616233 8.199291

41 H 3.735181 8.538510 9.950387 7.616233 8.383981

42 H 2.748162 7.988172 9.825697 9.046227 9.627240

43 H 4.948707 1.094133 3.739802 12.147558 11.608272

44 H 4.948707 1.094133 3.739802 12.147558 11.739540

45 H 6.362094 1.090799 2.732916 12.789864 12.147558

36 37 38 39 40

36 H 0.000000

37 H 8.395108 0.000000

38 H 8.210668 1.749489 0.000000

39 H 7.654731 1.773517 1.773517 0.000000

40 H 8.383981 11.598918 11.730116 12.166458 0.000000

41 H 8.199291 11.730116 11.598918 12.166458 1.749489

42 H 9.627240 12.166458 12.166458 12.835128 1.773517

43 H 11.739540 8.199291 8.383981 9.627240 8.210668

44 H 11.608272 8.383981 8.199291 9.627240 8.395108

45 H 12.147558 7.616233 7.616233 9.046227 9.621908

41 42 43 44 45

41 H 0.000000

42 H 1.773517 0.000000

43 H 8.395108 7.654731 0.000000

44 H 8.210668 7.654731 1.750664 0.000000

45 H 9.621908 9.073387 1.770750 1.770750 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=0 Diff= 7.23D-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 2.805157 -1.110434 0.000000

2 7 0 2.011097 0.001373 0.000000

3 6 0 2.789824 1.114109 0.000000

4 6 0 4.196951 0.691828 0.000000

5 6 0 4.187464 -0.681879 0.000000

6 7 0 2.380427 2.416890 0.000000

7 6 0 1.114985 2.796873 0.000000

8 7 0 0.000000 2.005123 0.000000

9 6 0 -1.120812 2.782911 0.000000

10 6 0 -0.683594 4.221507 0.000000

11 6 0 0.665500 4.208544 0.000000

12 7 0 2.383247 -2.414341 0.000000

13 6 0 0.683594 -4.221507 0.000000

14 6 0 -0.665500 -4.208544 0.000000

15 6 0 -1.114985 -2.796873 0.000000

16 7 0 -0.000000 -2.005123 0.000000

17 6 0 1.120812 -2.782911 0.000000

18 7 0 -2.380427 -2.416890 0.000000

19 7 0 -2.011097 -0.001373 0.000000

20 6 0 -2.789824 -1.114109 0.000000

21 6 0 -4.196951 -0.691828 0.000000

22 6 0 -4.187464 0.681879 0.000000

23 6 0 -2.805157 1.110434 0.000000

24 7 0 -2.383247 2.414341 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 5.356703 1.623930 0.000000

27 1 0 5.042650 -1.343848 0.000000

28 6 0 -1.629751 5.366468 0.000000

29 1 0 1.335301 5.056012 0.000000

30 6 0 1.629751 -5.366468 0.000000

31 1 0 -1.335301 -5.056012 0.000000

32 6 0 -5.356703 -1.623930 0.000000

33 1 0 -5.042650 1.343848 0.000000

34 1 0 6.302876 1.081160 0.000000

35 1 0 5.337524 2.280095 0.875332

36 1 0 5.337524 2.280095 -0.875332

37 1 0 -2.285651 5.330059 0.874744

38 1 0 -2.285651 5.330059 -0.874744

39 1 0 -1.103944 6.321902 0.000000

40 1 0 2.285651 -5.330059 0.874744

41 1 0 2.285651 -5.330059 -0.874744

42 1 0 1.103944 -6.321902 0.000000

43 1 0 -5.337524 -2.280095 0.875332

44 1 0 -5.337524 -2.280095 -0.875332

45 1 0 -6.302876 -1.081160 0.000000

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

Rotational constants (GHZ): 0.1828691 0.1816318 0.0913275

Leave Link 202 at Tue Sep 17 14:23:07 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 101 beta electrons

nuclear repulsion energy 2760.5077531963 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= -0.1142361248 Hartrees.

Nuclear repulsion after empirical dispersion term = 2760.3935170715 Hartrees.

No density basis found on file 724.

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Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 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 = 3494

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.20D-06

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 124

GePol: Fraction of low-weight points (<1% of avg) = 3.55%

GePol: Cavity surface area = 382.218 Ang\*\*2

GePol: Cavity volume = 379.350 Ang\*\*3

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

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PCM non-electrostatic energy = -0.0107069466 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2760.3828101249 Hartrees.

Leave Link 301 at Tue Sep 17 14:23:07 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= 15323 LenP2D= 41248.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.85D-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 14:23:07 2019, MaxMem= 2415919104 cpu: 13.9

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:23:08 2019, MaxMem= 2415919104 cpu: 1.4

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= -0.000000 -0.000000 0.000000

Rot= 1.000000 -0.000000 0.000000 -0.000330 Ang= -0.04 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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(AG) (BU) (BU) (AG) (AG) (AU) (BG) (BG) (AG) (BU)

(AU) (BU) (AG) (AU) (BG) (BG) (AG) (AG) (AU) (BU)

(BU) (AU) (AG) (BU) (BU) (AG) (AG) (BG) (BU) (BU)

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The electronic state of the initial guess is 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0181 S= 1.0060

Leave Link 401 at Tue Sep 17 14:23:09 2019, MaxMem= 2415919104 cpu: 21.9

(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= 36624108.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.55D-15 for 3491.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.89D-15 for 2518 220.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.00D-15 for 3491.

Iteration 1 A^-1\*A deviation from orthogonality is 3.11D-12 for 1756 1746.

E= -1275.84235033736

DIIS: error= 3.38D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.84235033736 IErMin= 1 ErrMin= 3.38D-04

ErrMax= 3.38D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.80D-04 BMatP= 6.80D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.38D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.303 Goal= None Shift= 0.000

Gap= 0.393 Goal= None Shift= 0.000

RMSDP=4.07D-05 MaxDP=1.11D-03 OVMax= 7.72D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.07D-05 CP: 1.00D+00

E= -1275.84256908671 Delta-E= -0.000218749349 Rises=F Damp=F

DIIS: error= 1.90D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84256908671 IErMin= 2 ErrMin= 1.90D-04

ErrMax= 1.90D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.62D-05 BMatP= 6.80D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.90D-03

Coeff-Com: 0.938D-01 0.906D+00

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

Coeff: 0.937D-01 0.906D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.32D-05 MaxDP=6.33D-04 DE=-2.19D-04 OVMax= 6.70D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.27D-05 CP: 1.00D+00 1.09D+00

E= -1275.84257040355 Delta-E= -0.000001316841 Rises=F Damp=F

DIIS: error= 2.71D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1275.84257040355 IErMin= 2 ErrMin= 1.90D-04

ErrMax= 2.71D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.69D-05 BMatP= 5.62D-05

IDIUse=3 WtCom= 3.78D-01 WtEn= 6.22D-01

Coeff-Com: -0.149D-01 0.546D+00 0.469D+00

Coeff-En: 0.000D+00 0.479D+00 0.521D+00

Coeff: -0.564D-02 0.504D+00 0.501D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=7.13D-06 MaxDP=3.56D-04 DE=-1.32D-06 OVMax= 1.43D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 6.07D-06 CP: 1.00D+00 1.12D+00 7.15D-01

E= -1275.84258901190 Delta-E= -0.000018608353 Rises=F Damp=F

DIIS: error= 1.37D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84258901190 IErMin= 4 ErrMin= 1.37D-04

ErrMax= 1.37D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.65D-06 BMatP= 5.62D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.37D-03

Coeff-Com: -0.101D-01 0.157D+00 0.253D+00 0.600D+00

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

Coeff: -0.101D-01 0.157D+00 0.253D+00 0.600D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.29D-06 MaxDP=2.39D-04 DE=-1.86D-05 OVMax= 2.99D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.85D-06 CP: 1.00D+00 1.14D+00 9.44D-01 1.17D+00

E= -1275.84259186187 Delta-E= -0.000002849962 Rises=F Damp=F

DIIS: error= 7.58D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84259186187 IErMin= 5 ErrMin= 7.58D-05

ErrMax= 7.58D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.89D-06 BMatP= 5.65D-06

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

Coeff-Com: -0.338D-02 0.110D-01 0.834D-01 0.421D+00 0.488D+00

Coeff: -0.338D-02 0.110D-01 0.834D-01 0.421D+00 0.488D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.67D-06 MaxDP=1.13D-04 DE=-2.85D-06 OVMax= 1.86D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 9.59D-07 CP: 1.00D+00 1.16D+00 1.05D+00 1.48D+00 1.11D+00

E= -1275.84259335381 Delta-E= -0.000001491947 Rises=F Damp=F

DIIS: error= 5.85D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84259335381 IErMin= 6 ErrMin= 5.85D-05

ErrMax= 5.85D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.86D-07 BMatP= 1.89D-06

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

Coeff-Com: 0.507D-02-0.857D-01-0.117D+00-0.971D-01-0.448D-01 0.134D+01

Coeff: 0.507D-02-0.857D-01-0.117D+00-0.971D-01-0.448D-01 0.134D+01

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=5.90D-06 MaxDP=3.09D-04 DE=-1.49D-06 OVMax= 4.56D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 9.08D-07 CP: 1.00D+00 1.19D+00 1.31D+00 2.11D+00 1.94D+00

CP: 2.03D+00

E= -1275.84259544222 Delta-E= -0.000002088402 Rises=F Damp=F

DIIS: error= 3.80D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84259544222 IErMin= 7 ErrMin= 3.80D-05

ErrMax= 3.80D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.73D-07 BMatP= 4.86D-07

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

Coeff-Com: 0.607D-02-0.676D-01-0.144D+00-0.305D+00-0.478D+00 0.109D+01

Coeff-Com: 0.897D+00

Coeff: 0.607D-02-0.676D-01-0.144D+00-0.305D+00-0.478D+00 0.109D+01

Coeff: 0.897D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=5.86D-06 MaxDP=2.99D-04 DE=-2.09D-06 OVMax= 4.48D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 7.18D-07 CP: 1.00D+00 1.23D+00 1.57D+00 2.75D+00 2.68D+00

CP: 3.00D+00 1.65D+00

E= -1275.84259676393 Delta-E= -0.000001321711 Rises=F Damp=F

DIIS: error= 1.86D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84259676393 IErMin= 8 ErrMin= 1.86D-05

ErrMax= 1.86D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.54D-08 BMatP= 4.73D-07

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

Coeff-Com: -0.111D-02 0.364D-01 0.246D-01-0.472D-02-0.208D+00-0.270D+00

Coeff-Com: 0.219D+00 0.120D+01

Coeff: -0.111D-02 0.364D-01 0.246D-01-0.472D-02-0.208D+00-0.270D+00

Coeff: 0.219D+00 0.120D+01

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.94D-06 MaxDP=2.05D-04 DE=-1.32D-06 OVMax= 3.04D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.34D-06 CP: 1.00D+00 1.25D+00 1.73D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.43D+00 2.32D+00

E= -1275.84259716964 Delta-E= -0.000000405711 Rises=F Damp=F

DIIS: error= 7.32D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84259716964 IErMin= 9 ErrMin= 7.32D-06

ErrMax= 7.32D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.30D-08 BMatP= 9.54D-08

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

Coeff-Com: -0.200D-02 0.367D-01 0.481D-01 0.746D-01-0.321D-02-0.403D+00

Coeff-Com: -0.135D+00 0.683D+00 0.701D+00

Coeff: -0.200D-02 0.367D-01 0.481D-01 0.746D-01-0.321D-02-0.403D+00

Coeff: -0.135D+00 0.683D+00 0.701D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.33D-06 MaxDP=7.05D-05 DE=-4.06D-07 OVMax= 1.01D-03

Cycle 10 Pass 1 IDiag 1:

RMSU= 3.64D-07 CP: 1.00D+00 1.26D+00 1.78D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.74D+00 2.91D+00 1.67D+00

E= -1275.84259722717 Delta-E= -0.000000057532 Rises=F Damp=F

DIIS: error= 2.62D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84259722717 IErMin=10 ErrMin= 2.62D-06

ErrMax= 2.62D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.96D-09 BMatP= 4.30D-08

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

Coeff-Com: -0.753D-03 0.781D-02 0.180D-01 0.453D-01 0.646D-01-0.113D+00

Coeff-Com: -0.155D+00-0.263D-01 0.367D+00 0.793D+00

Coeff: -0.753D-03 0.781D-02 0.180D-01 0.453D-01 0.646D-01-0.113D+00

Coeff: -0.155D+00-0.263D-01 0.367D+00 0.793D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.35D-07 MaxDP=2.47D-05 DE=-5.75D-08 OVMax= 3.22D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.50D-07 CP: 1.00D+00 1.26D+00 1.80D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.88D+00 3.00D+00 1.89D+00 1.16D+00

E= -1275.84259723684 Delta-E= -0.000000009666 Rises=F Damp=F

DIIS: error= 1.47D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84259723684 IErMin=11 ErrMin= 1.47D-06

ErrMax= 1.47D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.47D-09 BMatP= 8.96D-09

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

Coeff-Com: 0.203D-04-0.340D-02-0.714D-03 0.982D-02 0.297D-01 0.229D-01

Coeff-Com: -0.556D-01-0.139D+00 0.483D-01 0.419D+00 0.670D+00

Coeff: 0.203D-04-0.340D-02-0.714D-03 0.982D-02 0.297D-01 0.229D-01

Coeff: -0.556D-01-0.139D+00 0.483D-01 0.419D+00 0.670D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.59D-07 MaxDP=7.40D-06 DE=-9.67D-09 OVMax= 1.12D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 6.90D-08 CP: 1.00D+00 1.26D+00 1.80D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.91D+00 3.00D+00 1.97D+00 1.26D+00

CP: 1.27D+00

E= -1275.84259723881 Delta-E= -0.000000001974 Rises=F Damp=F

DIIS: error= 6.56D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84259723881 IErMin=12 ErrMin= 6.56D-07

ErrMax= 6.56D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.43D-10 BMatP= 2.47D-09

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

Coeff-Com: 0.174D-03-0.343D-02-0.475D-02-0.528D-02-0.427D-02 0.383D-01

Coeff-Com: 0.853D-02-0.620D-01-0.680D-01 0.148D-01 0.341D+00 0.745D+00

Coeff: 0.174D-03-0.343D-02-0.475D-02-0.528D-02-0.427D-02 0.383D-01

Coeff: 0.853D-02-0.620D-01-0.680D-01 0.148D-01 0.341D+00 0.745D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.23D-07 MaxDP=6.41D-06 DE=-1.97D-09 OVMax= 9.14D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 2.72D-08 CP: 1.00D+00 1.26D+00 1.81D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.93D+00 3.00D+00 2.03D+00 1.33D+00

CP: 1.52D+00 1.22D+00

E= -1275.84259723954 Delta-E= -0.000000000733 Rises=F Damp=F

DIIS: error= 4.41D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84259723954 IErMin=13 ErrMin= 4.41D-07

ErrMax= 4.41D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.56D-10 BMatP= 6.43D-10

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

Coeff-Com: 0.802D-04-0.512D-03-0.193D-02-0.451D-02-0.119D-01 0.115D-01

Coeff-Com: 0.194D-01 0.140D-01-0.437D-01-0.119D+00-0.578D-01 0.315D+00

Coeff-Com: 0.880D+00

Coeff: 0.802D-04-0.512D-03-0.193D-02-0.451D-02-0.119D-01 0.115D-01

Coeff: 0.194D-01 0.140D-01-0.437D-01-0.119D+00-0.578D-01 0.315D+00

Coeff: 0.880D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=5.34D-08 MaxDP=2.57D-06 DE=-7.33D-10 OVMax= 3.47D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 1.84D-08 CP: 1.00D+00 1.26D+00 1.81D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.94D+00 3.00D+00 2.06D+00 1.36D+00

CP: 1.66D+00 1.45D+00 1.29D+00

E= -1275.84259723973 Delta-E= -0.000000000185 Rises=F Damp=F

DIIS: error= 2.58D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84259723973 IErMin=14 ErrMin= 2.58D-07

ErrMax= 2.58D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.23D-11 BMatP= 1.56D-10

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

Coeff-Com: -0.193D-04 0.964D-03 0.596D-03-0.744D-03-0.574D-02-0.750D-02

Coeff-Com: 0.806D-02 0.314D-01-0.116D-02-0.757D-01-0.152D+00-0.733D-01

Coeff-Com: 0.480D+00 0.795D+00

Coeff: -0.193D-04 0.964D-03 0.596D-03-0.744D-03-0.574D-02-0.750D-02

Coeff: 0.806D-02 0.314D-01-0.116D-02-0.757D-01-0.152D+00-0.733D-01

Coeff: 0.480D+00 0.795D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.12D-08 MaxDP=1.67D-06 DE=-1.85D-10 OVMax= 1.97D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 8.22D-09 CP: 1.00D+00 1.26D+00 1.81D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.95D+00 3.00D+00 2.07D+00 1.38D+00

CP: 1.73D+00 1.58D+00 1.67D+00 1.28D+00

E= -1275.84259723980 Delta-E= -0.000000000078 Rises=F Damp=F

DIIS: error= 1.29D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.84259723980 IErMin=15 ErrMin= 1.29D-07

ErrMax= 1.29D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.37D-11 BMatP= 5.23D-11

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

Coeff-Com: -0.256D-04 0.563D-03 0.716D-03 0.578D-03 0.216D-03-0.609D-02

Coeff-Com: -0.272D-03 0.110D-01 0.902D-02-0.104D-01-0.614D-01-0.100D+00

Coeff-Com: 0.324D-01 0.404D+00 0.720D+00

Coeff: -0.256D-04 0.563D-03 0.716D-03 0.578D-03 0.216D-03-0.609D-02

Coeff: -0.272D-03 0.110D-01 0.902D-02-0.104D-01-0.614D-01-0.100D+00

Coeff: 0.324D-01 0.404D+00 0.720D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=7.62D-09 MaxDP=5.82D-07 DE=-7.78D-11 OVMax= 3.27D-06

Error on total polarization charges = 0.06462

SCF Done: E(UB3LYP) = -1275.84259724 A.U. after 15 cycles

NFock= 15 Conv=0.76D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0179 S= 1.0059

<L.S>= 0.000000000000E+00

KE= 1.320795439612D+03 PE=-8.572700268408D+03 EE= 3.215679421432D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.72

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0179, after 2.0002

Leave Link 502 at Tue Sep 17 14:24:28 2019, MaxMem= 2415919104 cpu: 1390.6

(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= 41248.

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 = 248

Leave Link 701 at Tue Sep 17 14:24:32 2019, MaxMem= 2415919104 cpu: 70.6

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 14:24:32 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 14:24:42 2019, MaxMem= 2415919104 cpu: 176.3

(Enter /home/blab/g09/l716.exe)

Dipole =-2.04281037D-13-1.99840144D-14-6.66133815D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000332166 -0.001491775 0.000000000

2 7 0.000635669 0.000283638 0.000000000

3 6 -0.002571216 0.000317884 -0.000000000

4 6 0.001197420 -0.000275754 -0.000000000

5 6 -0.000346429 0.001055740 0.000000000

6 7 -0.001092880 0.000330451 0.000000000

7 6 0.000897898 0.001702933 0.000000000

8 7 -0.001328280 0.000524404 0.000000000

9 6 0.000690158 -0.002398029 0.000000000

10 6 -0.000016442 -0.000146033 -0.000000000

11 6 0.000210425 -0.000530466 0.000000000

12 7 0.001860198 -0.001489516 -0.000000000

13 6 0.000016442 0.000146033 -0.000000000

14 6 -0.000210425 0.000530466 0.000000000

15 6 -0.000897898 -0.001702933 0.000000000

16 7 0.001328280 -0.000524404 -0.000000000

17 6 -0.000690158 0.002398029 0.000000000

18 7 0.001092880 -0.000330451 -0.000000000

19 7 -0.000635669 -0.000283638 -0.000000000

20 6 0.002571216 -0.000317884 0.000000000

21 6 -0.001197420 0.000275754 -0.000000000

22 6 0.000346429 -0.001055740 -0.000000000

23 6 -0.000332166 0.001491775 0.000000000

24 7 -0.001860198 0.001489516 0.000000000

25 30 -0.000000000 0.000000000 0.000000000

26 6 0.000134380 -0.000112661 0.000000000

27 1 0.000158034 0.000182427 0.000000000

28 6 -0.000069890 0.000219944 0.000000000

29 1 0.000352350 -0.000714399 -0.000000000

30 6 0.000069890 -0.000219944 -0.000000000

31 1 -0.000352350 0.000714399 0.000000000

32 6 -0.000134380 0.000112661 0.000000000

33 1 -0.000158034 -0.000182427 0.000000000

34 1 -0.000292550 -0.000203585 0.000000000

35 1 0.000249213 -0.000097826 0.000684919

36 1 0.000249213 -0.000097826 -0.000684919

37 1 -0.000048385 0.000130901 0.000647220

38 1 -0.000048385 0.000130901 -0.000647220

39 1 -0.000041995 -0.000328377 0.000000000

40 1 0.000048385 -0.000130901 0.000647220

41 1 0.000048385 -0.000130901 -0.000647220

42 1 0.000041995 0.000328377 0.000000000

43 1 -0.000249213 0.000097826 0.000684919

44 1 -0.000249213 0.000097826 -0.000684919

45 1 0.000292550 0.000203585 -0.000000000

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

Cartesian Forces: Max 0.002571216 RMS 0.000715447

Leave Link 716 at Tue Sep 17 14:24:42 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 0.001580085 RMS 0.000415635

Search for a local minimum.

Step number 20 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 12 13 14 15

16 17 18 19 20

DE= -4.47D-05 DEPred=-1.49D-04 R= 2.99D-01

Trust test= 2.99D-01 RLast= 4.84D-02 DXMaxT set to 8.41D-02

ITU= 0 1 -1 -1 1 1 -1 1 1 1 -1 0 1 -1 1 1 1 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.00951

Eigenvalues --- 0.01337 0.01338 0.01345 0.01346 0.01605

Eigenvalues --- 0.01623 0.01632 0.01640 0.01774 0.01793

Eigenvalues --- 0.01809 0.01823 0.01891 0.01911 0.01940

Eigenvalues --- 0.01951 0.01997 0.02000 0.02045 0.02048

Eigenvalues --- 0.02070 0.02087 0.02103 0.02111 0.02115

Eigenvalues --- 0.02205 0.02312 0.02316 0.02350 0.02372

Eigenvalues --- 0.06920 0.07167 0.07167 0.07182 0.07182

Eigenvalues --- 0.07310 0.07359 0.07384 0.10357 0.14073

Eigenvalues --- 0.14498 0.14499 0.14980 0.15345 0.15836

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16015 0.16164 0.16305 0.18185 0.20574

Eigenvalues --- 0.21379 0.22062 0.22094 0.23055 0.23839

Eigenvalues --- 0.23840 0.23853 0.24713 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25058

Eigenvalues --- 0.26006 0.27316 0.29645 0.30819 0.31364

Eigenvalues --- 0.33195 0.33202 0.33282 0.33282 0.33393

Eigenvalues --- 0.33698 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33724 0.33980 0.34375 0.34432

Eigenvalues --- 0.34437 0.34437 0.34612 0.35423 0.35552

Eigenvalues --- 0.35559 0.35641 0.35682 0.35682 0.36310

Eigenvalues --- 0.38666 0.39374 0.41638 0.41811 0.44173

Eigenvalues --- 0.45511 0.46813 0.48971 0.48986 0.51207

Eigenvalues --- 0.51358 0.51361 0.53675 0.54028 0.54033

Eigenvalues --- 0.54308 0.56319 0.56326 0.57434

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 0.45377 0.77353 -0.22730

Cosine: 0.995 > 0.840

Length: 1.017

GDIIS step was calculated using 3 of the last 20 vectors.

Iteration 1 RMS(Cart)= 0.00299968 RMS(Int)= 0.00000395

Iteration 2 RMS(Cart)= 0.00000912 RMS(Int)= 0.00000189

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000189

ITry= 1 IFail=0 DXMaxC= 1.04D-02 DCOld= 1.00D+10 DXMaxT= 8.41D-02 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.22D-09 for atom 29.

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

(Linear) (Quad) (Total)

R1 2.58184 -0.00096 0.00104 -0.00864 -0.00760 2.57425

R2 2.73484 -0.00057 -0.00108 0.00286 0.00178 2.73662

R3 2.58981 -0.00060 -0.00364 0.00155 -0.00210 2.58771

R4 2.56655 -0.00135 -0.00369 0.00714 0.00345 2.57000

R5 3.80042 -0.00005 0.00134 -0.00523 -0.00388 3.79654

R6 2.77624 -0.00081 -0.00093 -0.00430 -0.00524 2.77100

R7 2.58060 -0.00065 -0.00197 -0.00177 -0.00374 2.57685

R8 2.59599 0.00032 0.00079 0.00148 0.00226 2.59825

R9 2.81172 0.00059 0.00161 0.00046 0.00207 2.81379

R10 2.04365 -0.00023 -0.00058 0.00067 0.00009 2.04375

R11 2.49682 0.00025 0.00308 -0.00482 -0.00175 2.49507

R12 2.58420 -0.00068 -0.00222 0.00665 0.00443 2.58863

R13 2.79963 0.00026 -0.00073 -0.00238 -0.00311 2.79652

R14 2.57806 -0.00066 0.00075 -0.00711 -0.00636 2.57170

R15 3.78913 -0.00084 -0.00058 -0.00770 -0.00828 3.78086

R16 2.84133 0.00033 -0.00260 0.00232 -0.00027 2.84106

R17 2.48525 0.00158 0.00377 0.00153 0.00530 2.49055

R18 2.54954 0.00018 0.00187 0.00104 0.00290 2.55244

R19 2.80683 -0.00015 -0.00020 0.00182 0.00162 2.80845

R20 2.04129 0.00080 0.00160 0.00002 0.00162 2.04291

R21 2.48525 0.00158 0.00377 0.00153 0.00530 2.49055

R22 2.54954 0.00018 0.00187 0.00104 0.00290 2.55244

R23 2.84133 0.00033 -0.00260 0.00232 -0.00027 2.84106

R24 2.80683 -0.00015 -0.00020 0.00182 0.00162 2.80845

R25 2.79963 0.00026 -0.00073 -0.00238 -0.00311 2.79652

R26 2.04129 0.00080 0.00160 0.00002 0.00162 2.04291

R27 2.58420 -0.00068 -0.00222 0.00665 0.00443 2.58863

R28 2.49682 0.00025 0.00308 -0.00482 -0.00175 2.49507

R29 2.57806 -0.00066 0.00075 -0.00711 -0.00636 2.57170

R30 3.78913 -0.00084 -0.00058 -0.00770 -0.00828 3.78086

R31 2.58060 -0.00065 -0.00197 -0.00177 -0.00374 2.57685

R32 2.56655 -0.00135 -0.00369 0.00714 0.00345 2.57000

R33 2.58184 -0.00096 0.00104 -0.00864 -0.00760 2.57425

R34 3.80042 -0.00005 0.00134 -0.00523 -0.00388 3.79654

R35 2.77624 -0.00081 -0.00093 -0.00430 -0.00524 2.77100

R36 2.59599 0.00032 0.00079 0.00148 0.00226 2.59825

R37 2.81172 0.00059 0.00161 0.00046 0.00207 2.81379

R38 2.73484 -0.00057 -0.00108 0.00286 0.00178 2.73662

R39 2.04365 -0.00023 -0.00058 0.00067 0.00009 2.04375

R40 2.58981 -0.00060 -0.00364 0.00155 -0.00210 2.58771

R41 2.06131 0.00036 0.00070 0.00069 0.00139 2.06271

R42 2.06761 0.00071 0.00126 0.00143 0.00269 2.07031

R43 2.06761 0.00071 0.00126 0.00143 0.00269 2.07031

R44 2.06725 0.00058 0.00082 0.00196 0.00277 2.07002

R45 2.06725 0.00058 0.00082 0.00196 0.00277 2.07002

R46 2.06086 0.00023 0.00041 0.00090 0.00131 2.06217

R47 2.06725 0.00058 0.00082 0.00196 0.00277 2.07002

R48 2.06725 0.00058 0.00082 0.00196 0.00277 2.07002

R49 2.06086 0.00023 0.00041 0.00090 0.00131 2.06217

R50 2.06761 0.00071 0.00126 0.00143 0.00269 2.07031

R51 2.06761 0.00071 0.00126 0.00143 0.00269 2.07031

R52 2.06131 0.00036 0.00070 0.00069 0.00139 2.06271

A1 1.89036 0.00056 0.00015 0.00331 0.00347 1.89383

A2 2.20845 -0.00076 -0.00199 0.00015 -0.00184 2.20661

A3 2.18437 0.00020 0.00184 -0.00345 -0.00162 2.18275

A4 1.91078 -0.00078 -0.00116 -0.00345 -0.00461 1.90618

A5 2.19031 0.00041 0.00026 0.00335 0.00361 2.19392

A6 2.18209 0.00037 0.00091 0.00009 0.00100 2.18309

A7 1.88986 0.00134 0.00254 0.00294 0.00548 1.89534

A8 2.22650 -0.00060 -0.00137 -0.00392 -0.00528 2.22122

A9 2.16682 -0.00074 -0.00117 0.00098 -0.00020 2.16662

A10 1.85544 -0.00102 -0.00170 -0.00196 -0.00366 1.85178

A11 2.17305 0.00029 -0.00037 0.00362 0.00326 2.17630

A12 2.25470 0.00072 0.00206 -0.00166 0.00041 2.25511

A13 1.87833 -0.00010 0.00016 -0.00084 -0.00068 1.87766

A14 2.18224 -0.00003 -0.00090 0.00054 -0.00036 2.18188

A15 2.22262 0.00013 0.00074 0.00029 0.00104 2.22365

A16 2.16698 0.00075 0.00205 0.00369 0.00574 2.17272

A17 2.23241 -0.00057 -0.00156 -0.00137 -0.00294 2.22947

A18 2.17076 -0.00034 -0.00066 0.00052 -0.00013 2.17063

A19 1.88001 0.00092 0.00222 0.00085 0.00307 1.88308

A20 1.91747 -0.00047 -0.00161 -0.00172 -0.00333 1.91414

A21 2.18827 0.00015 0.00013 -0.00072 -0.00060 2.18767

A22 2.17745 0.00032 0.00148 0.00244 0.00392 2.18137

A23 1.88240 0.00036 0.00106 0.00233 0.00340 1.88580

A24 2.25088 -0.00103 -0.00440 0.00144 -0.00296 2.24792

A25 2.14990 0.00067 0.00334 -0.00377 -0.00043 2.14947

A26 1.85624 0.00003 0.00016 -0.00062 -0.00045 1.85579

A27 2.15593 -0.00017 0.00059 -0.00107 -0.00049 2.15544

A28 2.27102 0.00013 -0.00075 0.00169 0.00094 2.27196

A29 1.88866 -0.00084 -0.00184 -0.00085 -0.00269 1.88597

A30 2.16450 0.00037 0.00112 -0.00030 0.00083 2.16533

A31 2.23002 0.00047 0.00071 0.00115 0.00186 2.23188

A32 2.16779 0.00097 0.00451 -0.00515 -0.00064 2.16715

A33 1.85624 0.00003 0.00016 -0.00062 -0.00045 1.85579

A34 2.27102 0.00013 -0.00075 0.00169 0.00094 2.27196

A35 2.15593 -0.00017 0.00059 -0.00107 -0.00049 2.15544

A36 1.88866 -0.00084 -0.00184 -0.00085 -0.00269 1.88597

A37 2.23002 0.00047 0.00071 0.00115 0.00186 2.23188

A38 2.16450 0.00037 0.00112 -0.00030 0.00083 2.16533

A39 1.88001 0.00092 0.00222 0.00085 0.00307 1.88308

A40 2.17076 -0.00034 -0.00066 0.00052 -0.00013 2.17063

A41 2.23241 -0.00057 -0.00156 -0.00137 -0.00294 2.22947

A42 1.91747 -0.00047 -0.00161 -0.00172 -0.00333 1.91414

A43 2.18827 0.00015 0.00013 -0.00072 -0.00060 2.18767

A44 2.17745 0.00032 0.00148 0.00244 0.00392 2.18137

A45 2.14990 0.00067 0.00334 -0.00377 -0.00043 2.14947

A46 2.25088 -0.00103 -0.00440 0.00144 -0.00296 2.24792

A47 1.88240 0.00036 0.00106 0.00233 0.00340 1.88580

A48 2.16698 0.00075 0.00205 0.00369 0.00574 2.17272

A49 1.91078 -0.00078 -0.00116 -0.00345 -0.00461 1.90618

A50 2.18209 0.00037 0.00091 0.00009 0.00100 2.18309

A51 2.19031 0.00041 0.00026 0.00335 0.00361 2.19392

A52 2.22650 -0.00060 -0.00137 -0.00392 -0.00528 2.22122

A53 2.16682 -0.00074 -0.00117 0.00098 -0.00020 2.16662

A54 1.88986 0.00134 0.00254 0.00294 0.00548 1.89534

A55 1.85544 -0.00102 -0.00170 -0.00196 -0.00366 1.85178

A56 2.17305 0.00029 -0.00037 0.00362 0.00326 2.17630

A57 2.25470 0.00072 0.00206 -0.00166 0.00041 2.25511

A58 1.87833 -0.00010 0.00016 -0.00084 -0.00068 1.87766

A59 2.22262 0.00013 0.00074 0.00029 0.00104 2.22365

A60 2.18224 -0.00003 -0.00090 0.00054 -0.00036 2.18188

A61 1.89036 0.00056 0.00015 0.00331 0.00347 1.89383

A62 2.20845 -0.00076 -0.00199 0.00015 -0.00184 2.20661

A63 2.18437 0.00020 0.00184 -0.00345 -0.00162 2.18275

A64 2.16779 0.00097 0.00451 -0.00515 -0.00064 2.16715

A65 1.57011 -0.00009 -0.00015 0.00224 0.00208 1.57220

A66 1.57148 0.00009 0.00015 -0.00224 -0.00208 1.56940

A67 1.57148 0.00009 0.00015 -0.00224 -0.00208 1.56940

A68 1.57011 -0.00009 -0.00015 0.00224 0.00208 1.57220

A69 1.94378 -0.00004 -0.00110 -0.00047 -0.00157 1.94221

A70 1.94124 -0.00009 -0.00015 -0.00088 -0.00103 1.94021

A71 1.94124 -0.00009 -0.00015 -0.00088 -0.00103 1.94021

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A73 1.88979 0.00000 -0.00020 -0.00007 -0.00027 1.88952

A74 1.85467 0.00022 0.00194 0.00252 0.00446 1.85913

A75 1.93508 -0.00018 -0.00064 -0.00025 -0.00089 1.93419

A76 1.93508 -0.00018 -0.00064 -0.00025 -0.00089 1.93419

A77 1.94788 -0.00031 -0.00270 0.00033 -0.00237 1.94551

A78 1.85335 0.00038 0.00347 0.00108 0.00454 1.85789

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A80 1.89467 0.00017 0.00041 -0.00044 -0.00003 1.89464

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D123 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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D125 1.03183 0.00008 0.00112 0.00101 0.00213 1.03396

D126 -1.03183 -0.00008 -0.00112 -0.00101 -0.00213 -1.03396

D127 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D128 -2.10976 0.00008 0.00112 0.00101 0.00213 -2.10763

D129 2.10976 -0.00008 -0.00112 -0.00101 -0.00213 2.10763

D130 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

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D135 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

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Item Value Threshold Converged?

Maximum Force 0.001580 0.000450 NO

RMS Force 0.000416 0.000300 NO

Maximum Displacement 0.010441 0.001800 NO

RMS Displacement 0.003004 0.001200 NO

Predicted change in Energy=-8.258601D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:24:42 2019, MaxMem= 2415919104 cpu: 1.3

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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1 6 0 -2.070576 -2.190635 0.000000

2 7 0 -0.747928 -1.864632 0.000000

3 6 0 -0.005993 -3.004413 0.000000

4 6 0 -0.915672 -4.154487 0.000000

5 6 0 -2.188286 -3.634002 0.000000

6 7 0 1.353949 -3.104391 0.000000

7 6 0 2.179340 -2.073851 0.000000

8 7 0 1.857971 -0.742238 0.000000

9 6 0 2.996187 0.003734 0.000000

10 6 0 4.169316 -0.936506 0.000000

11 6 0 3.654983 -2.185439 0.000000

12 7 0 -3.123786 -1.315483 0.000000

13 6 0 -4.169316 0.936506 0.000000

14 6 0 -3.654983 2.185439 0.000000

15 6 0 -2.179340 2.073851 0.000000

16 7 0 -1.857971 0.742238 0.000000

17 6 0 -2.996187 -0.003734 0.000000

18 7 0 -1.353949 3.104391 0.000000

19 7 0 0.747928 1.864632 0.000000

20 6 0 0.005993 3.004413 0.000000

21 6 0 0.915672 4.154487 0.000000

22 6 0 2.188286 3.634002 0.000000

23 6 0 2.070576 2.190635 0.000000

24 7 0 3.123786 1.315483 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.481227 -5.578690 0.000000

27 1 0 -3.121574 -4.180466 0.000000

28 6 0 5.584415 -0.482421 0.000000

29 1 0 4.191256 -3.124108 0.000000

30 6 0 -5.584415 0.482421 0.000000

31 1 0 -4.191256 3.124108 0.000000

32 6 0 0.481227 5.578690 0.000000

33 1 0 3.121574 4.180466 0.000000

34 1 0 -1.338494 -6.254370 0.000000

35 1 0 0.133949 -5.804601 0.877936

36 1 0 0.133949 -5.804601 -0.877936

37 1 0 5.793926 0.139012 0.877410

38 1 0 5.793926 0.139012 -0.877410

39 1 0 6.275012 -1.327353 0.000000

40 1 0 -5.793926 -0.139012 0.877410

41 1 0 -5.793926 -0.139012 -0.877410

42 1 0 -6.275012 1.327353 0.000000

43 1 0 -0.133949 5.804601 0.877936

44 1 0 -0.133949 5.804601 -0.877936

45 1 0 1.338494 6.254370 0.000000

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Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.362232 0.000000

3 C 2.219175 1.359988 0.000000

4 C 2.278271 2.295990 1.466351 0.000000

5 C 1.448158 2.281513 2.271296 1.374937 0.000000

6 N 3.544336 2.440264 1.363612 2.500775 3.581608

7 C 4.251520 2.934735 2.375211 3.729363 4.637912

8 N 4.187043 2.837336 2.931177 4.397333 4.973378

9 C 5.521534 4.184398 4.249945 5.709066 6.333394

10 C 6.364675 5.004069 4.659340 6.017683 6.906200

11 C 5.725561 4.414582 3.751461 4.976749 6.020143

12 N 1.369359 2.438497 3.545859 3.596625 2.500138

13 C 3.766129 4.421796 5.732722 6.041888 4.981368

14 C 4.654070 4.985383 6.344264 6.906409 6.001424

15 C 4.265873 4.190536 5.523785 6.355238 5.707860

16 N 2.940569 2.833367 4.179379 4.986566 4.388688

17 C 2.374720 2.918495 4.236194 4.642984 3.719079

18 N 5.343301 5.005842 6.255755 7.272097 6.789850

19 N 4.938538 4.018084 4.927068 6.244787 6.233484

20 C 5.594699 4.927068 6.008837 7.217985 6.991667

21 C 7.012720 6.244787 7.217985 8.508400 8.384218

22 C 7.215560 6.233484 6.991667 8.384218 8.484000

23 C 6.028654 4.938538 5.594699 7.012720 7.215560

24 N 6.266918 5.010320 5.334512 6.799838 7.260545

25 Zn 3.014327 2.009042 3.004419 4.254200 4.242000

26 C 3.742318 3.723621 2.617775 1.488991 2.587637

27 H 2.250339 3.316215 3.330157 2.206055 1.081503

28 C 7.843270 6.481441 6.132953 7.465601 8.387333

29 H 6.331028 5.097236 4.198956 5.209836 6.399887

30 C 4.415008 5.375897 6.578510 6.580127 5.336537

31 H 5.722218 6.061687 7.421267 7.981692 7.048684

32 C 8.177659 7.544128 8.596920 9.832907 9.591662

33 H 8.218841 7.177483 7.836081 9.261252 9.447779

34 H 4.129150 4.429285 3.512518 2.142029 2.754718

35 H 4.323361 4.131807 2.937926 2.143677 3.297734

36 H 4.323361 4.131807 2.937926 2.143677 3.297734

37 H 8.249090 6.897846 6.655075 8.013905 8.872496

38 H 8.249090 6.897846 6.655075 8.013905 8.872496

39 H 8.390118 7.043461 6.501042 7.726488 8.772003

40 H 4.340776 5.404601 6.517709 6.378969 5.097591

41 H 4.340776 5.404601 6.517709 6.378969 5.097591

42 H 5.482109 6.382588 7.620026 7.666361 6.427781

43 H 8.273155 7.743699 8.853579 10.028225 9.699396

44 H 8.273155 7.743699 8.853579 10.028225 9.699396

45 H 9.107133 8.382801 9.355891 10.650144 10.498479

6 7 8 9 10

6 N 0.000000

7 C 1.320335 0.000000

8 N 2.415328 1.369844 0.000000

9 C 3.515308 2.232397 1.360886 0.000000

10 C 3.553311 2.292064 2.319495 1.503424 0.000000

11 C 2.477747 1.479855 2.304795 2.286151 1.350693

12 N 4.821857 5.357077 5.014630 6.260544 7.302943

13 C 6.843633 7.026215 6.256706 7.225961 8.546401

14 C 7.285032 7.223633 6.242111 6.999850 8.424144

15 C 6.268838 6.016771 4.922422 5.574179 7.026215

16 N 5.011286 4.922422 4.001486 4.910014 6.256706

17 C 5.342075 5.574179 4.910014 5.992379 7.225961

18 N 6.773602 6.268838 5.011286 5.342075 6.843633

19 N 5.005842 4.190536 2.833367 2.918495 4.421796

20 C 6.255755 5.523785 4.179379 4.236194 5.732722

21 C 7.272097 6.355238 4.986566 4.642984 6.041888

22 C 6.789850 5.707860 4.388688 3.719079 4.981368

23 C 5.343301 4.265873 2.940569 2.374720 3.766129

24 N 4.761052 3.518460 2.415886 1.317941 2.482859

25 Zn 3.386801 3.008385 2.000743 2.996190 4.273201

26 C 3.080588 4.400285 5.372440 6.576918 6.570952

27 H 4.603069 5.704167 6.051221 7.411783 7.979997

28 C 4.977105 3.758615 3.735491 2.633490 1.486169

29 H 2.837376 2.269548 3.334296 3.348370 2.187712

30 C 7.810641 8.173764 7.542473 8.593944 9.856401

31 H 8.339275 8.222121 7.179260 7.835565 9.294502

32 C 8.726829 7.838684 6.469123 6.115976 7.486640

33 H 7.496242 6.324894 5.082294 4.178614 5.223138

34 H 4.143865 5.463689 6.371890 7.612708 7.656086

35 H 3.090356 4.344294 5.419459 6.534518 6.383831

36 H 3.090356 4.344294 5.419459 6.534518 6.383831

37 H 5.568026 4.328029 4.127734 2.935215 2.136807

38 H 5.568026 4.328029 4.127734 2.935215 2.136807

39 H 5.232086 4.163146 4.455627 3.538712 2.141661

40 H 7.788160 8.251450 7.725623 8.834948 10.033546

41 H 7.788160 8.251450 7.725623 8.834948 10.033546

42 H 8.822777 9.112862 8.392175 9.365207 10.686863

43 H 9.074952 8.257850 6.899247 6.649706 8.045582

44 H 9.074952 8.257850 6.899247 6.649706 8.045582

45 H 9.358774 8.370560 7.015866 6.466714 7.728017

11 12 13 14 15

11 C 0.000000

12 N 6.834364 0.000000

13 C 8.424144 2.482859 0.000000

14 C 8.517051 3.540992 1.350693 0.000000

15 C 7.223633 3.518460 2.292064 1.479855 0.000000

16 N 6.242111 2.415886 2.319495 2.304795 1.369844

17 C 6.999850 1.317941 1.503424 2.286151 2.232397

18 N 7.285032 4.761052 3.553311 2.477747 1.320335

19 N 4.985383 5.010320 5.004069 4.414582 2.934735

20 C 6.344264 5.334512 4.659340 3.751461 2.375211

21 C 6.906409 6.799838 6.017683 4.976749 3.729363

22 C 6.001424 7.260545 6.906200 6.020143 4.637912

23 C 4.654070 6.266918 6.364675 5.725561 4.251520

24 N 3.540992 6.778949 7.302943 6.834364 5.357077

25 Zn 4.258526 3.389474 4.273201 4.258526 3.008385

26 C 5.349989 5.015780 7.486640 8.387754 7.838684

27 H 7.064124 2.864984 5.223138 6.388213 6.324894

28 C 2.573515 8.747958 9.856401 9.616857 8.173764

29 H 1.081060 7.535315 9.294502 9.473899 8.222121

30 C 9.616857 3.047483 1.486169 2.573515 3.758615

31 H 9.473899 4.566121 2.187712 1.081060 2.269548

32 C 8.387754 7.779829 6.570952 5.349989 4.400285

33 H 6.388213 8.319254 7.979997 7.064124 5.704167

34 H 6.441352 5.251654 7.728017 8.751942 8.370560

35 H 5.125113 5.615674 8.045582 8.886366 8.257850

36 H 5.125113 5.615674 8.045582 8.886366 8.257850

37 H 3.278414 9.078050 10.033546 9.707707 8.251450

38 H 3.278414 9.078050 10.033546 9.707707 8.251450

39 H 2.756966 9.398805 10.686863 10.533019 9.112862

40 H 9.707707 3.046896 2.136807 3.278414 4.328029

41 H 9.707707 3.046896 2.136807 3.278414 4.328029

42 H 10.533019 4.112761 2.141661 2.756966 4.163146

43 H 8.886366 7.772097 6.383831 5.125113 4.344294

44 H 8.886366 7.772097 6.383831 5.125113 4.344294

45 H 8.751942 8.787185 7.656086 6.441352 5.463689

16 17 18 19 20

16 N 0.000000

17 C 1.360886 0.000000

18 N 2.415328 3.515308 0.000000

19 N 2.837336 4.184398 2.440264 0.000000

20 C 2.931177 4.249945 1.363612 1.359988 0.000000

21 C 4.397333 5.709066 2.500775 2.295990 1.466351

22 C 4.973378 6.333394 3.581608 2.281513 2.271296

23 C 4.187043 5.521534 3.544336 1.362232 2.219175

24 N 5.014630 6.260544 4.821857 2.438497 3.545859

25 Zn 2.000743 2.996190 3.386801 2.009042 3.004419

26 C 6.469123 6.115976 8.726829 7.544128 8.596920

27 H 5.082294 4.178614 7.496242 7.177483 7.836081

28 C 7.542473 8.593944 7.810641 5.375897 6.578510

29 H 7.179260 7.835565 8.339275 6.061687 7.421267

30 C 3.735491 2.633490 4.977105 6.481441 6.132953

31 H 3.334296 3.348370 2.837376 5.097236 4.198956

32 C 5.372440 6.576918 3.080588 3.723621 2.617775

33 H 6.051221 7.411783 4.603069 3.316215 3.330157

34 H 7.015866 6.466714 9.358774 8.382801 9.355891

35 H 6.899247 6.649706 9.074952 7.743699 8.853579

36 H 6.899247 6.649706 9.074952 7.743699 8.853579

37 H 7.725623 8.834948 7.788160 5.404601 6.517709

38 H 7.725623 8.834948 7.788160 5.404601 6.517709

39 H 8.392175 9.365207 8.822777 6.382588 7.620026

40 H 4.127734 2.935215 5.568026 6.897846 6.655075

41 H 4.127734 2.935215 5.568026 6.897846 6.655075

42 H 4.455627 3.538712 5.232086 7.043461 6.501042

43 H 5.419459 6.534518 3.090356 4.131807 2.937926

44 H 5.419459 6.534518 3.090356 4.131807 2.937926

45 H 6.371890 7.612708 4.143865 4.429285 3.512518

21 22 23 24 25

21 C 0.000000

22 C 1.374937 0.000000

23 C 2.278271 1.448158 0.000000

24 N 3.596625 2.500138 1.369359 0.000000

25 Zn 4.254200 4.242000 3.014327 3.389474 0.000000

26 C 9.832907 9.591662 8.177659 7.779829 5.599407

27 H 9.261252 9.447779 8.218841 8.319254 5.217329

28 C 6.580127 5.336537 4.415008 3.047483 5.605214

29 H 7.981692 7.048684 5.722218 4.566121 5.227493

30 C 7.465601 8.387333 7.843270 8.747958 5.605214

31 H 5.209836 6.399887 6.331028 7.535315 5.227493

32 C 1.488991 2.587637 3.742318 5.015780 5.599407

33 H 2.206055 1.081503 2.250339 2.864984 5.217329

34 H 10.650144 10.498479 9.107133 8.787185 6.395992

35 H 10.028225 9.699396 8.273155 7.772097 5.872146

36 H 10.028225 9.699396 8.273155 7.772097 5.872146

37 H 6.378969 5.097591 4.340776 3.046896 5.861633

38 H 6.378969 5.097591 4.340776 3.046896 5.861633

39 H 7.666361 6.427781 5.482109 4.112761 6.413863

40 H 8.013905 8.872496 8.249090 9.078050 5.861633

41 H 8.013905 8.872496 8.249090 9.078050 5.861633

42 H 7.726488 8.772003 8.390118 9.398805 6.413863

43 H 2.143677 3.297734 4.323361 5.615674 5.872146

44 H 2.143677 3.297734 4.323361 5.615674 5.872146

45 H 2.142029 2.754718 4.129150 5.251654 6.395992

26 27 28 29 30

26 C 0.000000

27 H 2.987719 0.000000

28 C 7.922371 9.458847 0.000000

29 H 5.277979 7.388733 2.986537 0.000000

30 C 7.923357 5.273338 11.210428 10.419731 0.000000

31 H 9.460603 7.382481 10.419731 10.454986 2.986537

32 C 11.198814 10.402946 7.923357 9.460603 7.922371

33 H 10.402946 10.434658 5.273338 7.382481 9.458847

34 H 1.091536 2.735041 9.013438 6.354265 7.963177

35 H 1.095558 3.742595 7.668373 4.941412 8.543834

36 H 1.095558 3.742595 7.668373 4.941412 8.543834

37 H 8.534606 9.945545 1.095409 3.739833 11.417286

38 H 8.534606 9.945545 1.095409 3.739833 11.417286

39 H 7.982519 9.820187 1.091254 2.751429 11.996720

40 H 7.654065 4.923887 11.417286 10.458705 1.095409

41 H 7.654065 4.923887 11.417286 10.458705 1.095409

42 H 9.014509 6.346672 11.996720 11.373578 1.091254

43 H 11.422376 10.459361 8.543834 9.959921 7.668373

44 H 11.422376 10.459361 8.543834 9.959921 7.668373

45 H 11.972163 11.348040 7.963177 9.802760 9.013438

31 32 33 34 35

31 H 0.000000

32 C 5.277979 0.000000

33 H 7.388733 2.987719 0.000000

34 H 9.802760 11.972163 11.348040 0.000000

35 H 9.959921 11.422376 10.459361 1.772330 0.000000

36 H 9.959921 11.422376 10.459361 1.772330 1.755871

37 H 10.458705 7.654065 4.923887 9.618555 8.207427

38 H 10.458705 7.654065 4.923887 9.618555 8.393039

39 H 11.373578 9.014509 6.346672 9.068680 7.650435

40 H 3.739833 8.534606 9.945545 7.616975 8.199914

41 H 3.739833 8.534606 9.945545 7.616975 8.385692

42 H 2.751429 7.982519 9.820187 9.047194 9.628620

43 H 4.941412 1.095558 3.742595 12.150739 11.612292

44 H 4.941412 1.095558 3.742595 12.150739 11.744293

45 H 6.354265 1.091536 2.735041 12.791983 12.150739

36 37 38 39 40

36 H 0.000000

37 H 8.393039 0.000000

38 H 8.207427 1.754820 0.000000

39 H 7.650435 1.775252 1.775252 0.000000

40 H 8.385692 11.591186 11.723267 12.158999 0.000000

41 H 8.199914 11.723267 11.591186 12.158999 1.754820

42 H 9.628620 12.158999 12.158999 12.827726 1.775252

43 H 11.744293 8.199914 8.385692 9.628620 8.207427

44 H 11.612292 8.385692 8.199914 9.628620 8.393039

45 H 12.150739 7.616975 7.616975 9.047194 9.618555

41 42 43 44 45

41 H 0.000000

42 H 1.775252 0.000000

43 H 8.393039 7.650435 0.000000

44 H 8.207427 7.650435 1.755871 0.000000

45 H 9.618555 9.068680 1.772330 1.772330 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=0 Diff= 1.39D-03

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 2.802457 -1.110136 0.000000

2 7 0 2.009040 -0.002812 0.000000

3 6 0 2.792242 1.109015 0.000000

4 6 0 4.197721 0.690907 0.000000

5 6 0 4.186494 -0.683985 0.000000

6 7 0 2.380574 2.409002 0.000000

7 6 0 1.117368 2.793183 0.000000

8 7 0 0.000000 2.000743 0.000000

9 6 0 -1.114996 2.780995 0.000000

10 6 0 -0.677060 4.219222 0.000000

11 6 0 0.673557 4.204921 0.000000

12 7 0 2.380477 -2.412855 0.000000

13 6 0 0.677060 -4.219222 0.000000

14 6 0 -0.673557 -4.204921 0.000000

15 6 0 -1.117368 -2.793183 0.000000

16 7 0 -0.000000 -2.000743 0.000000

17 6 0 1.114996 -2.780995 0.000000

18 7 0 -2.380574 -2.409002 0.000000

19 7 0 -2.009040 0.002812 0.000000

20 6 0 -2.792242 -1.109015 0.000000

21 6 0 -4.197721 -0.690907 0.000000

22 6 0 -4.186494 0.683985 0.000000

23 6 0 -2.802457 1.110136 0.000000

24 7 0 -2.380477 2.412855 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 5.359123 1.622702 0.000000

27 1 0 5.040195 -1.347946 0.000000

28 6 0 -1.623717 5.364882 0.000000

29 1 0 1.346296 5.051155 0.000000

30 6 0 1.623717 -5.364882 0.000000

31 1 0 -1.346296 -5.051155 0.000000

32 6 0 -5.359123 -1.622702 0.000000

33 1 0 -5.040195 1.347946 0.000000

34 1 0 6.304617 1.077273 0.000000

35 1 0 5.340694 2.277788 0.877936

36 1 0 5.340694 2.277788 -0.877936

37 1 0 -2.278529 5.328903 0.877410

38 1 0 -2.278529 5.328903 -0.877410

39 1 0 -1.095277 6.319652 0.000000

40 1 0 2.278529 -5.328903 0.877410

41 1 0 2.278529 -5.328903 -0.877410

42 1 0 1.095277 -6.319652 0.000000

43 1 0 -5.340694 -2.277788 0.877936

44 1 0 -5.340694 -2.277788 -0.877936

45 1 0 -6.304617 -1.077273 0.000000

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

Rotational constants (GHZ): 0.1828856 0.1819590 0.0914155

Leave Link 202 at Tue Sep 17 14:24:42 2019, MaxMem= 2415919104 cpu: 0.1

(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 101 beta electrons

nuclear repulsion energy 2761.7103271161 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= -0.1142058733 Hartrees.

Nuclear repulsion after empirical dispersion term = 2761.5961212428 Hartrees.

No density basis found on file 724.

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Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 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 = 3494

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.10D-06

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 134

GePol: Fraction of low-weight points (<1% of avg) = 3.84%

GePol: Cavity surface area = 382.072 Ang\*\*2

GePol: Cavity volume = 379.266 Ang\*\*3

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

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PCM non-electrostatic energy = -0.0107044167 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2761.5854168260 Hartrees.

Leave Link 301 at Tue Sep 17 14:24:42 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= 15325 LenP2D= 41258.

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 14:24:43 2019, MaxMem= 2415919104 cpu: 12.3

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:24:43 2019, MaxMem= 2415919104 cpu: 1.2

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= -0.000000 -0.000000 -0.000000

Rot= 1.000000 0.000000 -0.000000 0.000478 Ang= 0.05 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 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0179 S= 1.0059

Leave Link 401 at Tue Sep 17 14:24:44 2019, MaxMem= 2415919104 cpu: 21.9

(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= 36624108.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.11D-15 for 3491.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.89D-15 for 2610 2250.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.88D-15 for 3491.

Iteration 1 A^-1\*A deviation from orthogonality is 3.26D-11 for 1767 1745.

E= -1275.84248765200

DIIS: error= 3.80D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.84248765200 IErMin= 1 ErrMin= 3.80D-04

ErrMax= 3.80D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.76D-04 BMatP= 3.76D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.80D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.303 Goal= None Shift= 0.000

Gap= 0.393 Goal= None Shift= 0.000

RMSDP=3.14D-05 MaxDP=7.50D-04 OVMax= 7.92D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.14D-05 CP: 1.00D+00

E= -1275.84259812105 Delta-E= -0.000110469050 Rises=F Damp=F

DIIS: error= 1.55D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84259812105 IErMin= 2 ErrMin= 1.55D-04

ErrMax= 1.55D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.50D-05 BMatP= 3.76D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.55D-03

Coeff-Com: 0.161D+00 0.839D+00

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

Coeff: 0.160D+00 0.840D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.34D-05 MaxDP=5.54D-04 DE=-1.10D-04 OVMax= 7.04D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.32D-05 CP: 1.00D+00 1.07D+00

E= -1275.84259886623 Delta-E= -0.000000745176 Rises=F Damp=F

DIIS: error= 2.43D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1275.84259886623 IErMin= 2 ErrMin= 1.55D-04

ErrMax= 2.43D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.72D-05 BMatP= 5.50D-05

IDIUse=3 WtCom= 3.91D-01 WtEn= 6.09D-01

Coeff-Com: -0.654D-02 0.563D+00 0.443D+00

Coeff-En: 0.000D+00 0.489D+00 0.511D+00

Coeff: -0.256D-02 0.518D+00 0.485D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=8.31D-06 MaxDP=3.50D-04 DE=-7.45D-07 OVMax= 1.93D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 6.77D-06 CP: 1.00D+00 1.16D+00 6.93D-01

E= -1275.84261885324 Delta-E= -0.000019987010 Rises=F Damp=F

DIIS: error= 1.15D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84261885324 IErMin= 4 ErrMin= 1.15D-04

ErrMax= 1.15D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.38D-06 BMatP= 5.50D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.15D-03

Coeff-Com: -0.976D-02 0.193D+00 0.259D+00 0.558D+00

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

Coeff: -0.975D-02 0.192D+00 0.259D+00 0.559D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.38D-06 MaxDP=2.34D-04 DE=-2.00D-05 OVMax= 3.00D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.50D-06 CP: 1.00D+00 1.19D+00 9.41D-01 1.16D+00

E= -1275.84262237908 Delta-E= -0.000003525840 Rises=F Damp=F

DIIS: error= 7.63D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84262237908 IErMin= 5 ErrMin= 7.63D-05

ErrMax= 7.63D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.64D-06 BMatP= 6.38D-06

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

Coeff-Com: -0.928D-03-0.519D-01-0.954D-03 0.328D+00 0.726D+00

Coeff: -0.928D-03-0.519D-01-0.954D-03 0.328D+00 0.726D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.64D-06 MaxDP=2.14D-04 DE=-3.53D-06 OVMax= 3.40D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.02D-06 CP: 1.00D+00 1.24D+00 1.14D+00 1.62D+00 1.39D+00

E= -1275.84262512682 Delta-E= -0.000002747740 Rises=F Damp=F

DIIS: error= 6.41D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84262512682 IErMin= 6 ErrMin= 6.41D-05

ErrMax= 6.41D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.90D-07 BMatP= 1.64D-06

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

Coeff-Com: 0.658D-02-0.124D+00-0.160D+00-0.113D+00 0.130D+00 0.126D+01

Coeff: 0.658D-02-0.124D+00-0.160D+00-0.113D+00 0.130D+00 0.126D+01

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=7.45D-06 MaxDP=3.74D-04 DE=-2.75D-06 OVMax= 5.67D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.01D-06 CP: 1.00D+00 1.32D+00 1.46D+00 2.32D+00 2.44D+00

CP: 2.00D+00

E= -1275.84262807817 Delta-E= -0.000002951349 Rises=F Damp=F

DIIS: error= 4.58D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84262807817 IErMin= 7 ErrMin= 4.58D-05

ErrMax= 4.58D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.61D-07 BMatP= 6.90D-07

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

Coeff-Com: 0.697D-02-0.800D-01-0.170D+00-0.350D+00-0.524D+00 0.124D+01

Coeff-Com: 0.878D+00

Coeff: 0.697D-02-0.800D-01-0.170D+00-0.350D+00-0.524D+00 0.124D+01

Coeff: 0.878D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=8.43D-06 MaxDP=4.09D-04 DE=-2.95D-06 OVMax= 6.36D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.82D-06 CP: 1.00D+00 1.41D+00 1.82D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.50D+00

E= -1275.84262989827 Delta-E= -0.000001820100 Rises=F Damp=F

DIIS: error= 1.54D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84262989827 IErMin= 8 ErrMin= 1.54D-05

ErrMax= 1.54D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.31D-08 BMatP= 6.61D-07

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

Coeff-Com: 0.223D-03 0.294D-01 0.373D-02-0.453D-01-0.210D+00 0.389D-02

Coeff-Com: 0.277D+00 0.941D+00

Coeff: 0.223D-03 0.294D-01 0.373D-02-0.453D-01-0.210D+00 0.389D-02

Coeff: 0.277D+00 0.941D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.39D-06 MaxDP=1.31D-04 DE=-1.82D-06 OVMax= 1.85D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 8.41D-07 CP: 1.00D+00 1.43D+00 1.92D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.04D+00 1.91D+00

E= -1275.84263011928 Delta-E= -0.000000221012 Rises=F Damp=F

DIIS: error= 9.91D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84263011928 IErMin= 9 ErrMin= 9.91D-06

ErrMax= 9.91D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.17D-08 BMatP= 9.31D-08

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

Coeff-Com: -0.237D-02 0.488D-01 0.602D-01 0.954D-01 0.548D-01-0.433D+00

Coeff-Com: -0.151D+00 0.659D+00 0.668D+00

Coeff: -0.237D-02 0.488D-01 0.602D-01 0.954D-01 0.548D-01-0.433D+00

Coeff: -0.151D+00 0.659D+00 0.668D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.09D-06 MaxDP=6.00D-05 DE=-2.21D-07 OVMax= 8.08D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 2.56D-07 CP: 1.00D+00 1.43D+00 1.96D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.29D+00 2.35D+00 1.30D+00

E= -1275.84263019226 Delta-E= -0.000000072977 Rises=F Damp=F

DIIS: error= 4.21D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84263019226 IErMin=10 ErrMin= 4.21D-06

ErrMax= 4.21D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.79D-09 BMatP= 7.17D-08

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

Coeff-Com: -0.607D-03 0.349D-02 0.122D-01 0.408D-01 0.835D-01-0.114D+00

Coeff-Com: -0.153D+00-0.406D-01 0.133D+00 0.104D+01

Coeff: -0.607D-03 0.349D-02 0.122D-01 0.408D-01 0.835D-01-0.114D+00

Coeff: -0.153D+00-0.406D-01 0.133D+00 0.104D+01

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=6.68D-07 MaxDP=3.73D-05 DE=-7.30D-08 OVMax= 5.02D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.58D-07 CP: 1.00D+00 1.44D+00 1.98D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.48D+00 2.60D+00 1.51D+00 1.38D+00

E= -1275.84263021470 Delta-E= -0.000000022437 Rises=F Damp=F

DIIS: error= 2.90D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84263021470 IErMin=11 ErrMin= 2.90D-06

ErrMax= 2.90D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.03D-09 BMatP= 8.79D-09

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

Coeff-Com: 0.202D-03-0.105D-01-0.829D-02 0.366D-02 0.366D-01 0.467D-01

Coeff-Com: -0.723D-01-0.181D+00-0.122D+00 0.647D+00 0.660D+00

Coeff: 0.202D-03-0.105D-01-0.829D-02 0.366D-02 0.366D-01 0.467D-01

Coeff: -0.723D-01-0.181D+00-0.122D+00 0.647D+00 0.660D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.18D-07 MaxDP=1.71D-05 DE=-2.24D-08 OVMax= 2.33D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 7.39D-08 CP: 1.00D+00 1.44D+00 1.99D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.54D+00 2.72D+00 1.62D+00 1.72D+00

CP: 1.25D+00

E= -1275.84263022134 Delta-E= -0.000000006646 Rises=F Damp=F

DIIS: error= 1.31D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84263022134 IErMin=12 ErrMin= 1.31D-06

ErrMax= 1.31D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.43D-09 BMatP= 6.03D-09

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

Coeff-Com: 0.347D-03-0.657D-02-0.914D-02-0.118D-01-0.172D-01 0.701D-01

Coeff-Com: 0.977D-02-0.562D-01-0.127D+00-0.801D-01 0.304D+00 0.924D+00

Coeff: 0.347D-03-0.657D-02-0.914D-02-0.118D-01-0.172D-01 0.701D-01

Coeff: 0.977D-02-0.562D-01-0.127D+00-0.801D-01 0.304D+00 0.924D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.81D-07 MaxDP=1.50D-05 DE=-6.65D-09 OVMax= 2.15D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 4.12D-08 CP: 1.00D+00 1.44D+00 2.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.59D+00 2.82D+00 1.73D+00 1.93D+00

CP: 1.56D+00 1.15D+00

E= -1275.84263022387 Delta-E= -0.000000002532 Rises=F Damp=F

DIIS: error= 5.51D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84263022387 IErMin=13 ErrMin= 5.51D-07

ErrMax= 5.51D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.45D-10 BMatP= 1.43D-09

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

Coeff-Com: 0.155D-03-0.146D-02-0.363D-02-0.769D-02-0.200D-01 0.315D-01

Coeff-Com: 0.196D-01 0.123D-01-0.509D-01-0.198D+00 0.352D-01 0.556D+00

Coeff-Com: 0.627D+00

Coeff: 0.155D-03-0.146D-02-0.363D-02-0.769D-02-0.200D-01 0.315D-01

Coeff: 0.196D-01 0.123D-01-0.509D-01-0.198D+00 0.352D-01 0.556D+00

Coeff: 0.627D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.20D-07 MaxDP=6.01D-06 DE=-2.53D-09 OVMax= 9.08D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 2.06D-08 CP: 1.00D+00 1.45D+00 2.01D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.61D+00 2.87D+00 1.78D+00 2.00D+00

CP: 1.62D+00 1.37D+00 1.23D+00

E= -1275.84263022423 Delta-E= -0.000000000358 Rises=F Damp=F

DIIS: error= 2.08D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84263022423 IErMin=14 ErrMin= 2.08D-07

ErrMax= 2.08D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.02D-11 BMatP= 4.45D-10

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

Coeff-Com: -0.126D-04 0.117D-02 0.738D-03-0.401D-03-0.511D-02-0.445D-02

Coeff-Com: 0.660D-02 0.251D-01 0.105D-01-0.804D-01-0.678D-01 0.151D-01

Coeff-Com: 0.336D+00 0.763D+00

Coeff: -0.126D-04 0.117D-02 0.738D-03-0.401D-03-0.511D-02-0.445D-02

Coeff: 0.660D-02 0.251D-01 0.105D-01-0.804D-01-0.678D-01 0.151D-01

Coeff: 0.336D+00 0.763D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.74D-08 MaxDP=1.89D-06 DE=-3.58D-10 OVMax= 2.76D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 7.56D-09 CP: 1.00D+00 1.45D+00 2.01D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.61D+00 2.88D+00 1.80D+00 2.02D+00

CP: 1.66D+00 1.44D+00 1.45D+00 1.06D+00

E= -1275.84263022426 Delta-E= -0.000000000028 Rises=F Damp=F

DIIS: error= 7.70D-08 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.84263022426 IErMin=15 ErrMin= 7.70D-08

ErrMax= 7.70D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.26D-12 BMatP= 7.02D-11

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

Coeff-Com: -0.219D-04 0.640D-03 0.687D-03 0.518D-03-0.197D-04-0.517D-02

Coeff-Com: 0.120D-02 0.858D-02 0.914D-02-0.158D-01-0.310D-01-0.471D-01

Coeff-Com: 0.782D-01 0.290D+00 0.710D+00

Coeff: -0.219D-04 0.640D-03 0.687D-03 0.518D-03-0.197D-04-0.517D-02

Coeff: 0.120D-02 0.858D-02 0.914D-02-0.158D-01-0.310D-01-0.471D-01

Coeff: 0.782D-01 0.290D+00 0.710D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=6.26D-09 MaxDP=3.98D-07 DE=-2.77D-11 OVMax= 3.02D-06

Error on total polarization charges = 0.06466

SCF Done: E(UB3LYP) = -1275.84263022 A.U. after 15 cycles

NFock= 15 Conv=0.63D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0178 S= 1.0059

<L.S>= 0.000000000000E+00

KE= 1.320794058050D+03 PE=-8.575119149702D+03 EE= 3.216897044601D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.72

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0178, after 2.0002

Leave Link 502 at Tue Sep 17 14:26:03 2019, MaxMem= 2415919104 cpu: 1385.2

(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= 41258.

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 = 246

Leave Link 701 at Tue Sep 17 14:26:07 2019, MaxMem= 2415919104 cpu: 71.9

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 14:26:08 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 14:26:17 2019, MaxMem= 2415919104 cpu: 177.2

(Enter /home/blab/g09/l716.exe)

Dipole =-7.28306304D-14 1.09690035D-13-4.44089210D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.001355342 -0.000832599 0.000000000

2 7 0.001176524 -0.001550824 -0.000000000

3 6 -0.000629576 0.001140459 -0.000000000

4 6 -0.000759420 0.000190538 -0.000000000

5 6 0.000487672 0.000267042 0.000000000

6 7 0.000460839 -0.000634923 0.000000000

7 6 -0.000568566 0.000854233 0.000000000

8 7 -0.000144490 -0.001171715 0.000000000

9 6 0.000848344 0.001076152 0.000000000

10 6 0.000204006 -0.001147546 -0.000000000

11 6 0.000930820 0.000912085 0.000000000

12 7 0.000198515 0.000458997 -0.000000000

13 6 -0.000204006 0.001147546 0.000000000

14 6 -0.000930820 -0.000912085 -0.000000000

15 6 0.000568566 -0.000854233 0.000000000

16 7 0.000144490 0.001171715 0.000000000

17 6 -0.000848344 -0.001076152 -0.000000000

18 7 -0.000460839 0.000634923 0.000000000

19 7 -0.001176524 0.001550824 -0.000000000

20 6 0.000629576 -0.001140459 0.000000000

21 6 0.000759420 -0.000190538 -0.000000000

22 6 -0.000487672 -0.000267042 0.000000000

23 6 0.001355342 0.000832599 0.000000000

24 7 -0.000198515 -0.000458997 0.000000000

25 30 0.000000000 -0.000000000 0.000000000

26 6 0.000372241 0.000046661 -0.000000000

27 1 0.000185398 0.000209853 -0.000000000

28 6 -0.000167192 0.000142514 0.000000000

29 1 0.000057424 -0.000111026 0.000000000

30 6 0.000167192 -0.000142514 0.000000000

31 1 -0.000057424 0.000111026 -0.000000000

32 6 -0.000372241 -0.000046661 -0.000000000

33 1 -0.000185398 -0.000209853 0.000000000

34 1 0.000111968 0.000071878 0.000000000

35 1 -0.000096309 -0.000013297 -0.000305024

36 1 -0.000096309 -0.000013297 0.000305024

37 1 -0.000140423 -0.000199427 -0.000350477

38 1 -0.000140423 -0.000199427 0.000350477

39 1 -0.000195524 0.000101601 0.000000000

40 1 0.000140423 0.000199427 -0.000350477

41 1 0.000140423 0.000199427 0.000350477

42 1 0.000195524 -0.000101601 0.000000000

43 1 0.000096309 0.000013297 -0.000305024

44 1 0.000096309 0.000013297 0.000305024

45 1 -0.000111968 -0.000071878 -0.000000000

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

Cartesian Forces: Max 0.001550824 RMS 0.000517895

Leave Link 716 at Tue Sep 17 14:26:17 2019, MaxMem= 2415919104 cpu: 0.4

(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 0.001014047 RMS 0.000236032

Search for a local minimum.

Step number 21 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 12 13 14 15

16 17 18 19 20

21

DE= -3.30D-05 DEPred=-8.26D-05 R= 3.99D-01

Trust test= 3.99D-01 RLast= 3.76D-02 DXMaxT set to 8.41D-02

ITU= 0 0 1 -1 -1 1 1 -1 1 1 1 -1 0 1 -1 1 1 1 1 0

ITU= 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01335

Eigenvalues --- 0.01337 0.01345 0.01346 0.01604 0.01623

Eigenvalues --- 0.01631 0.01640 0.01774 0.01793 0.01809

Eigenvalues --- 0.01823 0.01889 0.01909 0.01939 0.01950

Eigenvalues --- 0.01997 0.02000 0.02045 0.02047 0.02070

Eigenvalues --- 0.02087 0.02102 0.02110 0.02115 0.02205

Eigenvalues --- 0.02312 0.02316 0.02351 0.02372 0.03972

Eigenvalues --- 0.07196 0.07196 0.07206 0.07206 0.07262

Eigenvalues --- 0.07315 0.07388 0.07484 0.08775 0.13349

Eigenvalues --- 0.14498 0.14500 0.14984 0.15764 0.15990

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16070 0.16226 0.16358 0.17677 0.19621

Eigenvalues --- 0.21586 0.22061 0.22091 0.22880 0.23841

Eigenvalues --- 0.23855 0.23990 0.24591 0.24995 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25745 0.27692 0.29752 0.31384 0.32915

Eigenvalues --- 0.33189 0.33197 0.33282 0.33282 0.33444

Eigenvalues --- 0.33690 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33724 0.33971 0.34423 0.34437

Eigenvalues --- 0.34437 0.34440 0.34731 0.34800 0.35555

Eigenvalues --- 0.35565 0.35650 0.35682 0.35682 0.35933

Eigenvalues --- 0.38665 0.39534 0.41641 0.41812 0.45328

Eigenvalues --- 0.46509 0.48465 0.48966 0.48979 0.51358

Eigenvalues --- 0.51362 0.51670 0.53720 0.54019 0.54024

Eigenvalues --- 0.54248 0.56324 0.56325 0.57134

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 0.43279 0.32185 0.24536

Cosine: 1.000 > 0.840

Length: 0.999

GDIIS step was calculated using 3 of the last 21 vectors.

Iteration 1 RMS(Cart)= 0.00290514 RMS(Int)= 0.00000531

Iteration 2 RMS(Cart)= 0.00001034 RMS(Int)= 0.00000086

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000086

ITry= 1 IFail=0 DXMaxC= 1.53D-02 DCOld= 1.00D+10 DXMaxT= 8.41D-02 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 4.00D-10 for atom 27.

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

(Linear) (Quad) (Total)

R1 2.57425 0.00096 0.00475 0.00273 0.00748 2.58172

R2 2.73662 -0.00060 -0.00197 -0.00091 -0.00288 2.73374

R3 2.58771 0.00024 -0.00194 0.00056 -0.00138 2.58633

R4 2.57000 -0.00101 -0.00410 -0.00439 -0.00849 2.56151

R5 3.79654 0.00048 0.00289 0.00092 0.00381 3.80035

R6 2.77100 -0.00003 0.00269 0.00314 0.00583 2.77683

R7 2.57685 0.00056 0.00088 0.00182 0.00270 2.57956

R8 2.59825 -0.00029 -0.00080 -0.00085 -0.00166 2.59660

R9 2.81379 -0.00000 -0.00083 0.00024 -0.00060 2.81319

R10 2.04375 -0.00027 -0.00021 -0.00025 -0.00046 2.04328

R11 2.49507 0.00030 0.00229 -0.00031 0.00198 2.49705

R12 2.58863 -0.00050 -0.00377 -0.00223 -0.00600 2.58263

R13 2.79652 0.00056 0.00140 0.00290 0.00430 2.80082

R14 2.57170 0.00076 0.00377 0.00158 0.00534 2.57704

R15 3.78086 0.00042 0.00436 -0.00081 0.00355 3.78441

R16 2.84106 0.00028 -0.00141 0.00294 0.00153 2.84259

R17 2.49055 -0.00015 -0.00159 -0.00113 -0.00272 2.48783

R18 2.55244 -0.00094 -0.00030 -0.00243 -0.00273 2.54971

R19 2.80845 -0.00066 -0.00087 -0.00072 -0.00159 2.80686

R20 2.04291 0.00013 -0.00037 0.00093 0.00056 2.04347

R21 2.49055 -0.00015 -0.00159 -0.00113 -0.00272 2.48783

R22 2.55244 -0.00094 -0.00030 -0.00243 -0.00273 2.54971

R23 2.84106 0.00028 -0.00141 0.00294 0.00153 2.84259

R24 2.80845 -0.00066 -0.00087 -0.00072 -0.00159 2.80686

R25 2.79652 0.00056 0.00140 0.00290 0.00430 2.80082

R26 2.04291 0.00013 -0.00037 0.00093 0.00056 2.04347

R27 2.58863 -0.00050 -0.00377 -0.00223 -0.00600 2.58263

R28 2.49507 0.00030 0.00229 -0.00031 0.00198 2.49705

R29 2.57170 0.00076 0.00377 0.00158 0.00534 2.57704

R30 3.78086 0.00042 0.00436 -0.00081 0.00355 3.78441

R31 2.57685 0.00056 0.00088 0.00182 0.00270 2.57956

R32 2.57000 -0.00101 -0.00410 -0.00439 -0.00849 2.56151

R33 2.57425 0.00096 0.00475 0.00273 0.00748 2.58172

R34 3.79654 0.00048 0.00289 0.00092 0.00381 3.80035

R35 2.77100 -0.00003 0.00269 0.00314 0.00583 2.77683

R36 2.59825 -0.00029 -0.00080 -0.00085 -0.00166 2.59660

R37 2.81379 -0.00000 -0.00083 0.00024 -0.00060 2.81319

R38 2.73662 -0.00060 -0.00197 -0.00091 -0.00288 2.73374

R39 2.04375 -0.00027 -0.00021 -0.00025 -0.00046 2.04328

R40 2.58771 0.00024 -0.00194 0.00056 -0.00138 2.58633

R41 2.06271 -0.00013 -0.00042 0.00021 -0.00020 2.06250

R42 2.07031 -0.00030 -0.00089 0.00031 -0.00058 2.06973

R43 2.07031 -0.00030 -0.00089 0.00031 -0.00058 2.06973

R44 2.07002 -0.00042 -0.00115 0.00010 -0.00105 2.06897

R45 2.07002 -0.00042 -0.00115 0.00010 -0.00105 2.06897

R46 2.06217 -0.00020 -0.00046 0.00002 -0.00045 2.06172

R47 2.07002 -0.00042 -0.00115 0.00010 -0.00105 2.06897

R48 2.07002 -0.00042 -0.00115 0.00010 -0.00105 2.06897

R49 2.06217 -0.00020 -0.00046 0.00002 -0.00045 2.06172

R50 2.07031 -0.00030 -0.00089 0.00031 -0.00058 2.06973

R51 2.07031 -0.00030 -0.00089 0.00031 -0.00058 2.06973

R52 2.06271 -0.00013 -0.00042 0.00021 -0.00020 2.06250

A1 1.89383 -0.00037 -0.00168 -0.00081 -0.00250 1.89133

A2 2.20661 -0.00002 0.00003 -0.00285 -0.00282 2.20379

A3 2.18275 0.00039 0.00166 0.00366 0.00532 2.18806

A4 1.90618 0.00024 0.00242 -0.00064 0.00178 1.90795

A5 2.19392 -0.00018 -0.00155 0.00023 -0.00132 2.19260

A6 2.18309 -0.00007 -0.00087 0.00041 -0.00045 2.18263

A7 1.89534 -0.00018 -0.00252 0.00223 -0.00030 1.89504

A8 2.22122 0.00032 0.00269 0.00068 0.00337 2.22459

A9 2.16662 -0.00014 -0.00017 -0.00291 -0.00308 2.16355

A10 1.85178 0.00023 0.00181 -0.00275 -0.00093 1.85085

A11 2.17630 -0.00050 -0.00308 -0.00106 -0.00414 2.17216

A12 2.25511 0.00027 0.00127 0.00381 0.00507 2.26018

A13 1.87766 0.00007 -0.00003 0.00198 0.00195 1.87960

A14 2.18188 -0.00013 -0.00044 -0.00161 -0.00205 2.17982

A15 2.22365 0.00005 0.00047 -0.00037 0.00010 2.22376

A16 2.17272 -0.00025 -0.00193 -0.00157 -0.00350 2.16922

A17 2.22947 0.00003 0.00086 0.00082 0.00168 2.23115

A18 2.17063 -0.00007 0.00036 -0.00262 -0.00226 2.16837

A19 1.88308 0.00003 -0.00122 0.00180 0.00058 1.88366

A20 1.91414 -0.00005 0.00143 -0.00020 0.00124 1.91538

A21 2.18767 0.00004 -0.00007 0.00036 0.00029 2.18796

A22 2.18137 0.00000 -0.00137 -0.00016 -0.00153 2.17984

A23 1.88580 -0.00029 -0.00113 -0.00152 -0.00265 1.88315

A24 2.24792 -0.00005 -0.00033 -0.00106 -0.00139 2.24653

A25 2.14947 0.00034 0.00146 0.00258 0.00404 2.15351

A26 1.85579 0.00024 -0.00027 0.00182 0.00155 1.85734

A27 2.15544 -0.00018 0.00018 -0.00290 -0.00272 2.15273

A28 2.27196 -0.00006 0.00009 0.00108 0.00117 2.27312

A29 1.88597 0.00007 0.00118 -0.00189 -0.00071 1.88526

A30 2.16533 -0.00004 -0.00030 -0.00042 -0.00072 2.16461

A31 2.23188 -0.00003 -0.00088 0.00231 0.00144 2.23332

A32 2.16715 0.00017 0.00254 0.00313 0.00567 2.17282

A33 1.85579 0.00024 -0.00027 0.00182 0.00155 1.85734

A34 2.27196 -0.00006 0.00009 0.00108 0.00117 2.27312

A35 2.15544 -0.00018 0.00018 -0.00290 -0.00272 2.15273

A36 1.88597 0.00007 0.00118 -0.00189 -0.00071 1.88526

A37 2.23188 -0.00003 -0.00088 0.00231 0.00144 2.23332

A38 2.16533 -0.00004 -0.00030 -0.00042 -0.00072 2.16461

A39 1.88308 0.00003 -0.00122 0.00180 0.00058 1.88366

A40 2.17063 -0.00007 0.00036 -0.00262 -0.00226 2.16837

A41 2.22947 0.00003 0.00086 0.00082 0.00168 2.23115

A42 1.91414 -0.00005 0.00143 -0.00020 0.00124 1.91538

A43 2.18767 0.00004 -0.00007 0.00036 0.00029 2.18796

A44 2.18137 0.00000 -0.00137 -0.00016 -0.00153 2.17984

A45 2.14947 0.00034 0.00146 0.00258 0.00404 2.15351

A46 2.24792 -0.00005 -0.00033 -0.00106 -0.00139 2.24653

A47 1.88580 -0.00029 -0.00113 -0.00152 -0.00265 1.88315

A48 2.17272 -0.00025 -0.00193 -0.00157 -0.00350 2.16922

A49 1.90618 0.00024 0.00242 -0.00064 0.00178 1.90795

A50 2.18309 -0.00007 -0.00087 0.00041 -0.00045 2.18263

A51 2.19392 -0.00018 -0.00155 0.00023 -0.00132 2.19260

A52 2.22122 0.00032 0.00269 0.00068 0.00337 2.22459

A53 2.16662 -0.00014 -0.00017 -0.00291 -0.00308 2.16355

A54 1.89534 -0.00018 -0.00252 0.00223 -0.00030 1.89504

A55 1.85178 0.00023 0.00181 -0.00275 -0.00093 1.85085

A56 2.17630 -0.00050 -0.00308 -0.00106 -0.00414 2.17216

A57 2.25511 0.00027 0.00127 0.00381 0.00507 2.26018

A58 1.87766 0.00007 -0.00003 0.00198 0.00195 1.87960

A59 2.22365 0.00005 0.00047 -0.00037 0.00010 2.22376

A60 2.18188 -0.00013 -0.00044 -0.00161 -0.00205 2.17982

A61 1.89383 -0.00037 -0.00168 -0.00081 -0.00250 1.89133

A62 2.20661 -0.00002 0.00003 -0.00285 -0.00282 2.20379

A63 2.18275 0.00039 0.00166 0.00366 0.00532 2.18806

A64 2.16715 0.00017 0.00254 0.00313 0.00567 2.17282

A65 1.57220 -0.00007 -0.00069 -0.00070 -0.00139 1.57080

A66 1.56940 0.00007 0.00069 0.00070 0.00139 1.57079

A67 1.56940 0.00007 0.00069 0.00070 0.00139 1.57079

A68 1.57220 -0.00007 -0.00069 -0.00070 -0.00139 1.57080

A69 1.94221 -0.00001 0.00050 0.00130 0.00180 1.94401

A70 1.94021 0.00011 0.00011 0.00032 0.00042 1.94063

A71 1.94021 0.00011 0.00011 0.00032 0.00042 1.94063

A72 1.88952 -0.00003 0.00006 -0.00028 -0.00022 1.88930

A73 1.88952 -0.00003 0.00006 -0.00028 -0.00022 1.88930

A74 1.85913 -0.00015 -0.00089 -0.00151 -0.00240 1.85672

A75 1.93419 -0.00005 -0.00017 0.00005 -0.00011 1.93408

A76 1.93419 -0.00005 -0.00017 0.00005 -0.00011 1.93408

A77 1.94551 -0.00009 0.00031 0.00006 0.00037 1.94588

A78 1.85789 0.00001 -0.00027 -0.00042 -0.00069 1.85720

A79 1.89464 0.00009 0.00014 0.00012 0.00025 1.89489

A80 1.89464 0.00009 0.00014 0.00012 0.00025 1.89489

A81 1.93419 -0.00005 -0.00017 0.00005 -0.00011 1.93408

A82 1.93419 -0.00005 -0.00017 0.00005 -0.00011 1.93408

A83 1.94551 -0.00009 0.00031 0.00006 0.00037 1.94588

A84 1.85789 0.00001 -0.00027 -0.00042 -0.00069 1.85720

A85 1.89464 0.00009 0.00014 0.00012 0.00025 1.89489

A86 1.89464 0.00009 0.00014 0.00012 0.00025 1.89489

A87 1.94021 0.00011 0.00011 0.00032 0.00042 1.94063

A88 1.94021 0.00011 0.00011 0.00032 0.00042 1.94063

A89 1.94221 -0.00001 0.00050 0.00130 0.00180 1.94401

A90 1.85913 -0.00015 -0.00089 -0.00151 -0.00240 1.85672

A91 1.88952 -0.00003 0.00006 -0.00028 -0.00022 1.88930

A92 1.88952 -0.00003 0.00006 -0.00028 -0.00022 1.88930

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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D120 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

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D123 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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D125 1.03396 -0.00002 -0.00049 -0.00074 -0.00123 1.03273

D126 -1.03396 0.00002 0.00049 0.00074 0.00123 -1.03273

D127 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D128 -2.10763 -0.00002 -0.00049 -0.00074 -0.00123 -2.10887

D129 2.10763 0.00002 0.00049 0.00074 0.00123 2.10887

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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 0.001014 0.000450 NO

RMS Force 0.000236 0.000300 YES

Maximum Displacement 0.015333 0.001800 NO

RMS Displacement 0.002903 0.001200 NO

Predicted change in Energy=-5.309507D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:26:18 2019, MaxMem= 2415919104 cpu: 1.4

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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1 6 0 -2.074797 -2.192457 0.000000

2 7 0 -0.747996 -1.866776 0.000000

3 6 0 -0.007582 -3.002184 0.000000

4 6 0 -0.918571 -4.155155 0.000000

5 6 0 -2.190162 -3.634483 0.000000

6 7 0 1.353527 -3.105744 0.000000

7 6 0 2.178598 -2.073607 0.000000

8 7 0 1.858951 -0.744846 0.000000

9 6 0 2.999154 0.003248 0.000000

10 6 0 4.170891 -0.940016 0.000000

11 6 0 3.656362 -2.187305 0.000000

12 7 0 -3.124134 -1.313803 0.000000

13 6 0 -4.170891 0.940016 0.000000

14 6 0 -3.656362 2.187305 0.000000

15 6 0 -2.178598 2.073607 0.000000

16 7 0 -1.858951 0.744846 0.000000

17 6 0 -2.999154 -0.003248 0.000000

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20 6 0 0.007582 3.002184 0.000000

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22 6 0 2.190162 3.634483 0.000000

23 6 0 2.074797 2.192457 0.000000

24 7 0 3.124134 1.313803 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.477581 -5.577014 0.000000

27 1 0 -3.123519 -4.180346 0.000000

28 6 0 5.584928 -0.485382 0.000000

29 1 0 4.190872 -3.127321 0.000000

30 6 0 -5.584928 0.485382 0.000000

31 1 0 -4.190872 3.127321 0.000000

32 6 0 0.477581 5.577014 0.000000

33 1 0 3.123519 4.180346 0.000000

34 1 0 -1.330380 -6.258152 0.000000

35 1 0 0.139548 -5.800107 0.876902

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37 1 0 5.793729 0.136257 0.876737

38 1 0 5.793729 0.136257 -0.876737

39 1 0 6.276170 -1.329482 0.000000

40 1 0 -5.793729 -0.136257 0.876737

41 1 0 -5.793729 -0.136257 -0.876737

42 1 0 -6.276170 1.329482 0.000000

43 1 0 -0.139548 5.800107 0.876902

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45 1 0 1.330380 6.258152 0.000000

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Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.366189 0.000000

3 C 2.220143 1.355493 0.000000

4 C 2.277947 2.294727 1.469436 0.000000

5 C 1.446632 2.281366 2.272324 1.374061 0.000000

6 N 3.547887 2.439557 1.365043 2.502737 3.582917

7 C 4.255056 2.933893 2.375213 3.731661 4.639223

8 N 4.191653 2.838115 2.929082 4.398276 4.974466

9 C 5.528662 4.187854 4.251245 5.713220 6.337356

10 C 6.370026 5.005430 4.659632 6.019945 6.908194

11 C 5.731162 4.416005 3.753467 4.980205 6.022969

12 N 1.368627 2.439633 3.544506 3.596914 2.501571

13 C 3.769085 4.426544 5.733592 6.044697 4.984910

14 C 4.656572 4.989405 6.343846 6.908133 6.003578

15 C 4.267327 4.192045 5.520594 6.354931 5.708101

16 N 2.945223 2.838096 4.179449 4.989421 4.391835

17 C 2.376358 2.922406 4.235932 4.644046 3.720260

18 N 5.347071 5.009254 6.254466 7.273915 6.791952

19 N 4.944243 4.022114 4.927237 6.248287 6.236715

20 C 5.596481 4.927237 6.004387 7.217011 6.991096

21 C 7.018008 6.248287 7.217011 8.510954 8.387054

22 C 7.221018 6.236715 6.991096 8.387054 8.486760

23 C 6.037103 4.944243 5.596481 7.018008 7.221018

24 N 6.270785 5.010935 5.332484 6.800953 7.261354

25 Zn 3.018552 2.011057 3.002193 4.255477 4.243380

26 C 3.742502 3.720079 2.617374 1.488675 2.589664

27 H 2.247558 3.315979 3.331235 2.205092 1.081260

28 C 7.847643 6.481834 6.132737 7.467445 8.388615

29 H 6.335029 5.097194 4.200319 5.211799 6.401157

30 C 4.414957 5.378528 6.577986 6.580993 5.338326

31 H 5.725191 6.065839 7.420967 7.983885 7.051584

32 C 8.177978 7.544007 8.592905 9.831803 9.590022

33 H 8.224057 7.180272 7.835338 9.263858 9.450225

34 H 4.133283 4.429826 3.514417 2.142938 2.760954

35 H 4.322894 4.126473 2.935809 2.143464 3.299460

36 H 4.322894 4.126473 2.935809 2.143464 3.299460

37 H 8.252593 6.897461 6.653848 8.014977 8.872973

38 H 8.252593 6.897461 6.653848 8.014977 8.872973

39 H 8.395438 7.044685 6.502574 7.729730 8.774497

40 H 4.339019 5.405811 6.516264 6.378666 5.098230

41 H 4.339019 5.405811 6.516264 6.378666 5.098230

42 H 5.482298 6.385670 7.619614 7.667145 6.429339

43 H 8.270141 7.740818 8.846846 10.024124 9.694609

44 H 8.270141 7.740818 8.846846 10.024124 9.694609

45 H 9.110875 8.386543 9.356493 10.653391 10.500402

6 7 8 9 10

6 N 0.000000

7 C 1.321381 0.000000

8 N 2.414393 1.366668 0.000000

9 C 3.517658 2.233078 1.363711 0.000000

10 C 3.553578 2.292217 2.320163 1.504232 0.000000

11 C 2.479229 1.482131 2.304642 2.287016 1.349248

12 N 4.822914 5.356889 5.015461 6.263328 7.304594

13 C 6.847435 7.028366 6.260811 7.230981 8.551014

14 C 7.288028 7.225104 6.246293 7.004713 8.428880

15 C 6.269097 6.015359 4.923970 5.576335 7.028366

16 N 5.014684 4.923970 4.005244 4.914382 6.260811

17 C 5.345214 5.576335 4.914382 5.998312 7.230981

18 N 6.775745 6.269097 5.014684 5.345214 6.847435

19 N 5.009254 4.192045 2.838096 2.922406 4.426544

20 C 6.254466 5.520594 4.179449 4.235932 5.733592

21 C 7.273915 6.354931 4.989421 4.644046 6.044697

22 C 6.791952 5.708101 4.391835 3.720260 4.984910

23 C 5.347071 4.267327 2.945223 2.376358 3.769085

24 N 4.761034 3.516900 2.416345 1.316501 2.485036

25 Zn 3.387872 3.007679 2.002622 2.999156 4.275507

26 C 3.075733 4.396492 5.367423 6.574725 6.565823

27 H 4.604206 5.705330 6.052080 7.415496 7.981739

28 C 4.977053 3.758397 3.735001 2.631537 1.485327

29 H 2.837427 2.271467 3.333773 3.349724 2.187396

30 C 7.812704 8.174397 7.544853 8.597612 9.859400

31 H 8.342150 8.223126 7.182899 7.839408 9.298512

32 C 8.726830 7.837439 6.471019 6.117614 7.490809

33 H 7.497998 6.324935 5.084943 4.178949 5.226385

34 H 4.140174 5.461075 6.369331 7.612490 7.651572

35 H 3.082579 4.337451 5.411189 6.528800 6.375042

36 H 3.082579 4.337451 5.411189 6.528800 6.375042

37 H 5.567282 4.326816 4.126438 2.931895 2.135565

38 H 5.567282 4.326816 4.126438 2.931895 2.135565

39 H 5.233309 4.164591 4.455740 3.537654 2.141001

40 H 7.789082 8.251060 7.726743 8.837586 10.035355

41 H 7.789082 8.251060 7.726743 8.837586 10.035355

42 H 8.825163 9.113952 8.395417 9.369661 10.690730

43 H 9.072618 8.254582 6.899229 6.650112 8.048484

44 H 9.072618 8.254582 6.899229 6.650112 8.048484

45 H 9.363924 8.374824 7.022917 6.473688 7.738354

11 12 13 14 15

11 C 0.000000

12 N 6.836529 0.000000

13 C 8.428880 2.485036 0.000000

14 C 8.521334 3.541331 1.349248 0.000000

15 C 7.225104 3.516900 2.292217 1.482131 0.000000

16 N 6.246293 2.416345 2.320163 2.304642 1.366668

17 C 7.004713 1.316501 1.504232 2.287016 2.233078

18 N 7.288028 4.761034 3.553578 2.479229 1.321381

19 N 4.989405 5.010935 5.005430 4.416005 2.933893

20 C 6.343846 5.332484 4.659632 3.753467 2.375213

21 C 6.908133 6.800953 6.019945 4.980205 3.731661

22 C 6.003578 7.261354 6.908194 6.022969 4.639223

23 C 4.656572 6.270785 6.370026 5.731162 4.255056

24 N 3.541331 6.778286 7.304594 6.836529 5.356889

25 Zn 4.260667 3.389143 4.275507 4.260667 3.007679

26 C 5.345990 5.017888 7.490809 8.389832 7.837439

27 H 7.066753 2.866543 5.226385 6.389906 6.324935

28 C 2.572142 8.748374 9.859400 9.620015 8.174397

29 H 1.081357 7.536455 9.298512 9.477570 8.223126

30 C 9.620015 3.048373 1.485327 2.572142 3.758397

31 H 9.477570 4.567441 2.187396 1.081357 2.271467

32 C 8.389832 7.775327 6.565823 5.345990 4.396492

33 H 6.389906 8.319786 7.981739 7.066753 5.705330

34 H 6.437344 5.259671 7.738354 8.759905 8.374824

35 H 5.117545 5.616716 8.048484 8.886880 8.254582

36 H 5.117545 5.616716 8.048484 8.886880 8.254582

37 H 3.276575 9.077423 10.035355 9.709773 8.251060

38 H 3.276575 9.077423 10.035355 9.709773 8.251060

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40 H 9.709773 3.046641 2.135565 3.276575 4.326816

41 H 9.709773 3.046641 2.135565 3.276575 4.326816

42 H 10.536744 4.113671 2.141001 2.756675 4.164591

43 H 8.886880 7.764304 6.375042 5.117545 4.337451

44 H 8.886880 7.764304 6.375042 5.117545 4.337451

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16 17 18 19 20

16 N 0.000000

17 C 1.363711 0.000000

18 N 2.414393 3.517658 0.000000

19 N 2.838115 4.187854 2.439557 0.000000

20 C 2.929082 4.251245 1.365043 1.355493 0.000000

21 C 4.398276 5.713220 2.502737 2.294727 1.469436

22 C 4.974466 6.337356 3.582917 2.281366 2.272324

23 C 4.191653 5.528662 3.547887 1.366189 2.220143

24 N 5.015461 6.263328 4.822914 2.439633 3.544506

25 Zn 2.002622 2.999156 3.387872 2.011057 3.002193

26 C 6.471019 6.117614 8.726830 7.544007 8.592905

27 H 5.084943 4.178949 7.497998 7.180272 7.835338

28 C 7.544853 8.597612 7.812704 5.378528 6.577986

29 H 7.182899 7.839408 8.342150 6.065839 7.420967

30 C 3.735001 2.631537 4.977053 6.481834 6.132737

31 H 3.333773 3.349724 2.837427 5.097194 4.200319

32 C 5.367423 6.574725 3.075733 3.720079 2.617374

33 H 6.052080 7.415496 4.604206 3.315979 3.331235

34 H 7.022917 6.473688 9.363924 8.386543 9.356493

35 H 6.899229 6.650112 9.072618 7.740818 8.846846

36 H 6.899229 6.650112 9.072618 7.740818 8.846846

37 H 7.726743 8.837586 7.789082 5.405811 6.516264

38 H 7.726743 8.837586 7.789082 5.405811 6.516264

39 H 8.395417 9.369661 8.825163 6.385670 7.619614

40 H 4.126438 2.931895 5.567282 6.897461 6.653848

41 H 4.126438 2.931895 5.567282 6.897461 6.653848

42 H 4.455740 3.537654 5.233309 7.044685 6.502574

43 H 5.411189 6.528800 3.082579 4.126473 2.935809

44 H 5.411189 6.528800 3.082579 4.126473 2.935809

45 H 6.369331 7.612490 4.140174 4.429826 3.514417

21 22 23 24 25

21 C 0.000000

22 C 1.374061 0.000000

23 C 2.277947 1.446632 0.000000

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25 Zn 4.255477 4.243380 3.018552 3.389143 0.000000

26 C 9.831803 9.590022 8.177978 7.775327 5.597425

27 H 9.263858 9.450225 8.224057 8.319786 5.218397

28 C 6.580993 5.338326 4.414957 3.048373 5.605981

29 H 7.983885 7.051584 5.725191 4.567441 5.229106

30 C 7.467445 8.388615 7.847643 8.748374 5.605981

31 H 5.211799 6.401157 6.335029 7.536455 5.229106

32 C 1.488675 2.589664 3.742502 5.017888 5.597425

33 H 2.205092 1.081260 2.247558 2.866543 5.218397

34 H 10.653391 10.500402 9.110875 8.785056 6.397998

35 H 10.024124 9.694609 8.270141 7.764304 5.867680

36 H 10.024124 9.694609 8.270141 7.764304 5.867680

37 H 6.378666 5.098230 4.339019 3.046641 5.861274

38 H 6.378666 5.098230 4.339019 3.046641 5.861274

39 H 7.667145 6.429339 5.482298 4.113671 6.415437

40 H 8.014977 8.872973 8.252593 9.077423 5.861274

41 H 8.014977 8.872973 8.252593 9.077423 5.861274

42 H 7.729730 8.774497 8.395438 9.400317 6.415437

43 H 2.143464 3.299460 4.322894 5.616716 5.867680

44 H 2.143464 3.299460 4.322894 5.616716 5.867680

45 H 2.142938 2.760954 4.133283 5.259671 6.397998

26 27 28 29 30

26 C 0.000000

27 H 2.991934 0.000000

28 C 7.916991 9.459906 0.000000

29 H 5.272139 7.389803 2.987179 0.000000

30 C 7.927019 5.275182 11.211962 10.421991 0.000000

31 H 9.463296 7.385204 10.421991 10.458212 2.987179

32 C 11.194850 10.400673 7.927019 9.463296 7.916991

33 H 10.400673 10.436793 5.275182 7.385204 9.459906

34 H 1.091428 2.744563 9.008128 6.347152 7.973483

35 H 1.095252 3.747024 7.659466 4.932136 8.546693

36 H 1.095252 3.747024 7.659466 4.932136 8.546693

37 H 8.528743 9.945805 1.094852 3.740155 11.417723

38 H 8.528743 9.945805 1.094852 3.740155 11.417723

39 H 7.978389 9.822504 1.091018 2.753306 11.999141

40 H 7.657149 4.924769 11.417723 10.459799 1.094852

41 H 7.657149 4.924769 11.417723 10.459799 1.094852

42 H 9.017944 6.348024 11.999141 11.376382 1.091018

43 H 11.415870 10.453826 8.546693 9.960947 7.659466

44 H 11.415870 10.453826 8.546693 9.960947 7.659466

45 H 11.972463 11.348985 7.973483 9.811703 9.008128

31 32 33 34 35

31 H 0.000000

32 C 5.272139 0.000000

33 H 7.389803 2.991934 0.000000

34 H 9.811703 11.972463 11.348985 0.000000

35 H 9.960947 11.415870 10.453826 1.771850 0.000000

36 H 9.960947 11.415870 10.453826 1.771850 1.753804

37 H 10.459799 7.657149 4.924769 9.613016 8.198181

38 H 10.459799 7.657149 4.924769 9.613016 8.383640

39 H 11.376382 9.017944 6.348024 9.063741 7.642877

40 H 3.740155 8.528743 9.945805 7.626779 8.202620

41 H 3.740155 8.528743 9.945805 7.626779 8.387981

42 H 2.753306 7.978389 9.822504 9.057208 9.631274

43 H 4.932136 1.095252 3.747024 12.148606 11.603570

44 H 4.932136 1.095252 3.747024 12.148606 11.735360

45 H 6.347152 1.091428 2.744563 12.795996 12.148606

36 37 38 39 40

36 H 0.000000

37 H 8.383640 0.000000

38 H 8.198181 1.753474 0.000000

39 H 7.642877 1.774770 1.774770 0.000000

40 H 8.387981 11.590662 11.722548 12.160383 0.000000

41 H 8.202620 11.722548 11.590662 12.160383 1.753474

42 H 9.631274 12.160383 12.160383 12.830874 1.774770

43 H 11.735360 8.202620 8.387981 9.631274 8.198181

44 H 11.603570 8.387981 8.202620 9.631274 8.383640

45 H 12.148606 7.626779 7.626779 9.057208 9.613016

41 42 43 44 45

41 H 0.000000

42 H 1.774770 0.000000

43 H 8.383640 7.642877 0.000000

44 H 8.198181 7.642877 1.753804 0.000000

45 H 9.613016 9.063741 1.771850 1.771850 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=0 Diff= 1.45D-03

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 2.806858 -1.110496 0.000000

2 7 0 2.011057 -0.000013 0.000000

3 6 0 2.789623 1.109580 0.000000

4 6 0 4.198707 0.692778 0.000000

5 6 0 4.188338 -0.681244 0.000000

6 7 0 2.379509 2.411559 0.000000

7 6 0 1.114546 2.793550 0.000000

8 7 0 0.000000 2.002622 0.000000

9 6 0 -1.118506 2.782783 0.000000

10 6 0 -0.678724 4.221291 0.000000

11 6 0 0.670454 4.207585 0.000000

12 7 0 2.381525 -2.411354 0.000000

13 6 0 0.678724 -4.221291 0.000000

14 6 0 -0.670454 -4.207585 0.000000

15 6 0 -1.114546 -2.793550 0.000000

16 7 0 -0.000000 -2.002622 0.000000

17 6 0 1.118506 -2.782783 0.000000

18 7 0 -2.379509 -2.411559 0.000000

19 7 0 -2.011057 0.000013 0.000000

20 6 0 -2.789623 -1.109580 0.000000

21 6 0 -4.198707 -0.692778 0.000000

22 6 0 -4.188338 0.681244 0.000000

23 6 0 -2.806858 1.110496 0.000000

24 7 0 -2.381525 2.411354 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 5.354540 1.630970 0.000000

27 1 0 5.042189 -1.344615 0.000000

28 6 0 -1.626673 5.364789 0.000000

29 1 0 1.344229 5.053375 0.000000

30 6 0 1.626673 -5.364789 0.000000

31 1 0 -1.344229 -5.053375 0.000000

32 6 0 -5.354540 -1.630970 0.000000

33 1 0 -5.042189 1.344615 0.000000

34 1 0 6.303999 1.092691 0.000000

35 1 0 5.332096 2.286802 0.876902

36 1 0 5.332096 2.286802 -0.876902

37 1 0 -2.281374 5.327400 0.876737

38 1 0 -2.281374 5.327400 -0.876737

39 1 0 -1.100227 6.320390 0.000000

40 1 0 2.281374 -5.327400 0.876737

41 1 0 2.281374 -5.327400 -0.876737

42 1 0 1.100227 -6.320390 0.000000

43 1 0 -5.332096 -2.286802 0.876902

44 1 0 -5.332096 -2.286802 -0.876902

45 1 0 -6.303999 -1.092691 0.000000

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

Rotational constants (GHZ): 0.1828988 0.1818000 0.0913783

Leave Link 202 at Tue Sep 17 14:26:18 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 101 beta electrons

nuclear repulsion energy 2761.1865325653 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= -0.1142077945 Hartrees.

Nuclear repulsion after empirical dispersion term = 2761.0723247708 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 = 3498

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.47D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 130

GePol: Fraction of low-weight points (<1% of avg) = 3.72%

GePol: Cavity surface area = 382.234 Ang\*\*2

GePol: Cavity volume = 379.442 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0107288305 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2761.0615959403 Hartrees.

Leave Link 301 at Tue Sep 17 14:26:18 2019, MaxMem= 2415919104 cpu: 1.9

(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= 41260.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.85D-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 14:26:18 2019, MaxMem= 2415919104 cpu: 12.2

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:26:19 2019, MaxMem= 2415919104 cpu: 1.4

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= 0.000000 0.000000 -0.000000

Rot= 1.000000 -0.000000 -0.000000 -0.000419 Ang= -0.05 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 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0178 S= 1.0059

Leave Link 401 at Tue Sep 17 14:26:20 2019, MaxMem= 2415919104 cpu: 20.1

(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= 36708012.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.88D-15 for 3479.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.11D-15 for 3140 3066.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.88D-15 for 3479.

Iteration 1 A^-1\*A deviation from orthogonality is 2.37D-12 for 1770 1748.

E= -1275.84249253341

DIIS: error= 3.62D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.84249253341 IErMin= 1 ErrMin= 3.62D-04

ErrMax= 3.62D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.67D-04 BMatP= 3.67D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.62D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.303 Goal= None Shift= 0.000

Gap= 0.393 Goal= None Shift= 0.000

RMSDP=2.96D-05 MaxDP=7.76D-04 OVMax= 9.11D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.96D-05 CP: 1.00D+00

E= -1275.84263232445 Delta-E= -0.000139791045 Rises=F Damp=F

DIIS: error= 2.25D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84263232445 IErMin= 2 ErrMin= 2.25D-04

ErrMax= 2.25D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.81D-05 BMatP= 3.67D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.25D-03

Coeff-Com: 0.102D+00 0.898D+00

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

Coeff: 0.102D+00 0.898D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.46D-05 MaxDP=7.15D-04 DE=-1.40D-04 OVMax= 9.43D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.40D-05 CP: 1.00D+00 1.14D+00

E= -1275.84263342324 Delta-E= -0.000001098788 Rises=F Damp=F

DIIS: error= 3.75D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1275.84263342324 IErMin= 2 ErrMin= 2.25D-04

ErrMax= 3.75D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.29D-05 BMatP= 3.81D-05

IDIUse=3 WtCom= 3.40D-01 WtEn= 6.60D-01

Coeff-Com: -0.179D-01 0.613D+00 0.405D+00

Coeff-En: 0.000D+00 0.479D+00 0.521D+00

Coeff: -0.609D-02 0.525D+00 0.482D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=8.96D-06 MaxDP=4.48D-04 DE=-1.10D-06 OVMax= 2.23D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 7.54D-06 CP: 1.00D+00 1.23D+00 7.17D-01

E= -1275.84265245430 Delta-E= -0.000019031062 Rises=F Damp=F

DIIS: error= 1.80D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84265245430 IErMin= 4 ErrMin= 1.80D-04

ErrMax= 1.80D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.64D-06 BMatP= 3.81D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.80D-03

Coeff-Com: -0.110D-01 0.154D+00 0.269D+00 0.588D+00

Coeff-En: 0.000D+00 0.000D+00 0.195D-01 0.980D+00

Coeff: -0.110D-01 0.154D+00 0.269D+00 0.588D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=5.89D-06 MaxDP=3.17D-04 DE=-1.90D-05 OVMax= 4.10D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.40D-06 CP: 1.00D+00 1.29D+00 1.08D+00 1.06D+00

E= -1275.84265794942 Delta-E= -0.000005495117 Rises=F Damp=F

DIIS: error= 8.94D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84265794942 IErMin= 5 ErrMin= 8.94D-05

ErrMax= 8.94D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.39D-06 BMatP= 9.64D-06

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

Coeff-Com: 0.183D-02-0.957D-01-0.364D-02 0.376D+00 0.721D+00

Coeff: 0.183D-02-0.957D-01-0.364D-02 0.376D+00 0.721D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=5.75D-06 MaxDP=2.61D-04 DE=-5.50D-06 OVMax= 4.28D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.10D-06 CP: 1.00D+00 1.37D+00 1.34D+00 1.52D+00 1.33D+00

E= -1275.84266183265 Delta-E= -0.000003883226 Rises=F Damp=F

DIIS: error= 7.08D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84266183265 IErMin= 6 ErrMin= 7.08D-05

ErrMax= 7.08D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.04D-06 BMatP= 2.39D-06

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

Coeff-Com: 0.125D-01-0.155D+00-0.289D+00-0.307D+00 0.765D-01 0.166D+01

Coeff: 0.125D-01-0.155D+00-0.289D+00-0.307D+00 0.765D-01 0.166D+01

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.24D-05 MaxDP=6.17D-04 DE=-3.88D-06 OVMax= 9.45D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.10D-06 CP: 1.00D+00 1.54D+00 1.93D+00 2.43D+00 2.62D+00

CP: 2.63D+00

E= -1275.84266691872 Delta-E= -0.000005086076 Rises=F Damp=F

DIIS: error= 3.75D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84266691872 IErMin= 7 ErrMin= 3.75D-05

ErrMax= 3.75D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.79D-07 BMatP= 1.04D-06

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

Coeff-Com: 0.775D-02-0.660D-01-0.225D+00-0.374D+00-0.265D+00 0.117D+01

Coeff-Com: 0.753D+00

Coeff: 0.775D-02-0.660D-01-0.225D+00-0.374D+00-0.265D+00 0.117D+01

Coeff: 0.753D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=7.21D-06 MaxDP=3.59D-04 DE=-5.09D-06 OVMax= 5.47D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.45D-06 CP: 1.00D+00 1.64D+00 2.27D+00 2.96D+00 3.00D+00

CP: 3.00D+00 1.31D+00

E= -1275.84266818958 Delta-E= -0.000001270859 Rises=F Damp=F

DIIS: error= 1.19D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84266818958 IErMin= 8 ErrMin= 1.19D-05

ErrMax= 1.19D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.47D-07 BMatP= 5.79D-07

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

Coeff-Com: -0.214D-02 0.567D-01 0.353D-01 0.149D-01-0.980D-01-0.285D+00

Coeff-Com: 0.383D+00 0.895D+00

Coeff: -0.214D-02 0.567D-01 0.353D-01 0.149D-01-0.980D-01-0.285D+00

Coeff: 0.383D+00 0.895D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.82D-06 MaxDP=1.01D-04 DE=-1.27D-06 OVMax= 1.37D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 7.61D-07 CP: 1.00D+00 1.66D+00 2.35D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.73D+00 1.56D+00

E= -1275.84266836859 Delta-E= -0.000000179011 Rises=F Damp=F

DIIS: error= 7.23D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84266836859 IErMin= 9 ErrMin= 7.23D-06

ErrMax= 7.23D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.48D-08 BMatP= 1.47D-07

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

Coeff-Com: -0.295D-02 0.467D-01 0.670D-01 0.962D-01 0.302D-01-0.442D+00

Coeff-Com: 0.274D-01 0.480D+00 0.697D+00

Coeff: -0.295D-02 0.467D-01 0.670D-01 0.962D-01 0.302D-01-0.442D+00

Coeff: 0.274D-01 0.480D+00 0.697D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=6.39D-07 MaxDP=3.58D-05 DE=-1.79D-07 OVMax= 4.45D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 2.33D-07 CP: 1.00D+00 1.66D+00 2.37D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.89D+00 1.80D+00 1.31D+00

E= -1275.84266841341 Delta-E= -0.000000044814 Rises=F Damp=F

DIIS: error= 4.05D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84266841341 IErMin=10 ErrMin= 4.05D-06

ErrMax= 4.05D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.08D-08 BMatP= 4.48D-08

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

Coeff-Com: -0.336D-03-0.316D-02 0.861D-02 0.323D-01 0.565D-01-0.910D-01

Coeff-Com: -0.131D+00-0.834D-01 0.276D+00 0.935D+00

Coeff: -0.336D-03-0.316D-02 0.861D-02 0.323D-01 0.565D-01-0.910D-01

Coeff: -0.131D+00-0.834D-01 0.276D+00 0.935D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=7.36D-07 MaxDP=4.08D-05 DE=-4.48D-08 OVMax= 5.60D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.47D-07 CP: 1.00D+00 1.67D+00 2.40D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.04D+00 2.02D+00 1.78D+00 1.46D+00

E= -1275.84266843636 Delta-E= -0.000000022957 Rises=F Damp=F

DIIS: error= 2.33D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84266843636 IErMin=11 ErrMin= 2.33D-06

ErrMax= 2.33D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.64D-09 BMatP= 1.08D-08

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

Coeff-Com: 0.471D-03-0.123D-01-0.969D-02 0.311D-02 0.281D-01 0.479D-01

Coeff-Com: -0.958D-01-0.150D+00-0.454D-01 0.502D+00 0.731D+00

Coeff: 0.471D-03-0.123D-01-0.969D-02 0.311D-02 0.281D-01 0.479D-01

Coeff: -0.958D-01-0.150D+00-0.454D-01 0.502D+00 0.731D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.22D-07 MaxDP=1.12D-05 DE=-2.30D-08 OVMax= 1.44D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 7.41D-08 CP: 1.00D+00 1.67D+00 2.41D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.09D+00 2.08D+00 1.91D+00 1.83D+00

CP: 1.17D+00

E= -1275.84266844131 Delta-E= -0.000000004945 Rises=F Damp=F

DIIS: error= 1.32D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84266844131 IErMin=12 ErrMin= 1.32D-06

ErrMax= 1.32D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.65D-09 BMatP= 4.64D-09

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

Coeff-Com: 0.384D-03-0.556D-02-0.100D-01-0.114D-01-0.119D-01 0.631D-01

Coeff-Com: -0.519D-02-0.316D-01-0.143D+00-0.107D+00 0.421D+00 0.841D+00

Coeff: 0.384D-03-0.556D-02-0.100D-01-0.114D-01-0.119D-01 0.631D-01

Coeff: -0.519D-02-0.316D-01-0.143D+00-0.107D+00 0.421D+00 0.841D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.02D-07 MaxDP=1.54D-05 DE=-4.94D-09 OVMax= 2.30D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 3.92D-08 CP: 1.00D+00 1.68D+00 2.42D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.13D+00 2.15D+00 2.11D+00 2.11D+00

CP: 1.59D+00 9.35D-01

E= -1275.84266844376 Delta-E= -0.000000002453 Rises=F Damp=F

DIIS: error= 3.60D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84266844376 IErMin=13 ErrMin= 3.60D-07

ErrMax= 3.60D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.49D-10 BMatP= 1.65D-09

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

Coeff-Com: 0.772D-04 0.366D-03-0.255D-02-0.576D-02-0.132D-01 0.179D-01

Coeff-Com: 0.192D-01 0.246D-01-0.599D-01-0.180D+00 0.440D-01 0.415D+00

Coeff-Com: 0.741D+00

Coeff: 0.772D-04 0.366D-03-0.255D-02-0.576D-02-0.132D-01 0.179D-01

Coeff: 0.192D-01 0.246D-01-0.599D-01-0.180D+00 0.440D-01 0.415D+00

Coeff: 0.741D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.14D-07 MaxDP=5.62D-06 DE=-2.45D-09 OVMax= 8.57D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 2.13D-08 CP: 1.00D+00 1.68D+00 2.43D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.14D+00 2.18D+00 2.18D+00 2.22D+00

CP: 1.77D+00 1.01D+00 1.22D+00

E= -1275.84266844404 Delta-E= -0.000000000283 Rises=F Damp=F

DIIS: error= 1.96D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84266844404 IErMin=14 ErrMin= 1.96D-07

ErrMax= 1.96D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.21D-11 BMatP= 2.49D-10

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

Coeff-Com: -0.190D-04 0.126D-02 0.391D-03-0.113D-02-0.545D-02-0.996D-03

Coeff-Com: 0.126D-01 0.199D-01-0.101D-01-0.916D-01-0.516D-01 0.105D+00

Coeff-Com: 0.464D+00 0.557D+00

Coeff: -0.190D-04 0.126D-02 0.391D-03-0.113D-02-0.545D-02-0.996D-03

Coeff: 0.126D-01 0.199D-01-0.101D-01-0.916D-01-0.516D-01 0.105D+00

Coeff: 0.464D+00 0.557D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.23D-08 MaxDP=6.44D-07 DE=-2.83D-10 OVMax= 4.84D-06

Cycle 15 Pass 1 IDiag 1:

RMSU= 7.12D-09 CP: 1.00D+00 1.68D+00 2.43D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.14D+00 2.18D+00 2.19D+00 2.23D+00

CP: 1.79D+00 1.06D+00 1.28D+00 8.25D-01

E= -1275.84266844406 Delta-E= -0.000000000014 Rises=F Damp=F

DIIS: error= 8.01D-08 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.84266844406 IErMin=15 ErrMin= 8.01D-08

ErrMax= 8.01D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.75D-12 BMatP= 8.21D-11

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

Coeff-Com: -0.229D-04 0.498D-03 0.610D-03 0.274D-03-0.186D-03-0.358D-02

Coeff-Com: 0.310D-02 0.391D-02 0.643D-02-0.911D-02-0.351D-01-0.228D-01

Coeff-Com: 0.722D-01 0.222D+00 0.762D+00

Coeff: -0.229D-04 0.498D-03 0.610D-03 0.274D-03-0.186D-03-0.358D-02

Coeff: 0.310D-02 0.391D-02 0.643D-02-0.911D-02-0.351D-01-0.228D-01

Coeff: 0.722D-01 0.222D+00 0.762D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.88D-09 MaxDP=3.63D-07 DE=-1.36D-11 OVMax= 1.98D-06

Error on total polarization charges = 0.06466

SCF Done: E(UB3LYP) = -1275.84266844 A.U. after 15 cycles

NFock= 15 Conv=0.49D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0179 S= 1.0059

<L.S>= 0.000000000000E+00

KE= 1.320794494899D+03 PE=-8.574063621891D+03 EE= 3.216364862608D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.73

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0179, after 2.0002

Leave Link 502 at Tue Sep 17 14:27:39 2019, MaxMem= 2415919104 cpu: 1397.5

(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= 15325 LenP2D= 41260.

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 = 246

Leave Link 701 at Tue Sep 17 14:27:43 2019, MaxMem= 2415919104 cpu: 69.8

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 14:27:43 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 14:27:53 2019, MaxMem= 2415919104 cpu: 177.3

(Enter /home/blab/g09/l716.exe)

Dipole = 1.70530257D-13-7.06101844D-14-1.55431223D-15

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000404564 -0.000164847 0.000000000

2 7 0.000131821 0.000022163 0.000000000

3 6 -0.000432451 -0.000811614 -0.000000000

4 6 0.000987154 0.000850208 0.000000000

5 6 -0.000896336 0.000262293 0.000000000

6 7 0.000073818 -0.000097785 -0.000000000

7 6 0.000164521 -0.000116145 0.000000000

8 7 -0.000387631 -0.000022862 -0.000000000

9 6 0.000071564 -0.000363470 -0.000000000

10 6 0.000153423 0.000681493 -0.000000000

11 6 -0.000306686 -0.000011067 0.000000000

12 7 -0.000464217 -0.000201834 0.000000000

13 6 -0.000153423 -0.000681493 0.000000000

14 6 0.000306686 0.000011067 -0.000000000

15 6 -0.000164521 0.000116145 0.000000000

16 7 0.000387631 0.000022862 -0.000000000

17 6 -0.000071564 0.000363470 0.000000000

18 7 -0.000073818 0.000097785 -0.000000000

19 7 -0.000131821 -0.000022163 -0.000000000

20 6 0.000432451 0.000811614 0.000000000

21 6 -0.000987154 -0.000850208 -0.000000000

22 6 0.000896336 -0.000262293 -0.000000000

23 6 -0.000404564 0.000164847 0.000000000

24 7 0.000464217 0.000201834 0.000000000

25 30 0.000000000 -0.000000000 0.000000000

26 6 0.000022101 -0.000109322 0.000000000

27 1 0.000053361 -0.000005362 0.000000000

28 6 0.000184654 0.000001993 0.000000000

29 1 0.000006509 0.000112754 -0.000000000

30 6 -0.000184654 -0.000001993 -0.000000000

31 1 -0.000006509 -0.000112754 0.000000000

32 6 -0.000022101 0.000109322 0.000000000

33 1 -0.000053361 0.000005362 0.000000000

34 1 -0.000018181 0.000082282 0.000000000

35 1 -0.000067894 0.000047167 -0.000017249

36 1 -0.000067894 0.000047167 0.000017249

37 1 -0.000042868 -0.000051309 -0.000030305

38 1 -0.000042868 -0.000051309 0.000030305

39 1 -0.000060673 -0.000000603 0.000000000

40 1 0.000042868 0.000051309 -0.000030305

41 1 0.000042868 0.000051309 0.000030305

42 1 0.000060673 0.000000603 -0.000000000

43 1 0.000067894 -0.000047167 -0.000017249

44 1 0.000067894 -0.000047167 0.000017249

45 1 0.000018181 -0.000082282 -0.000000000

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

Cartesian Forces: Max 0.000987154 RMS 0.000269539

Leave Link 716 at Tue Sep 17 14:27:53 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 0.000738310 RMS 0.000129366

Search for a local minimum.

Step number 22 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 12 13 14 15

16 17 18 19 20

21 22

DE= -3.82D-05 DEPred=-5.31D-05 R= 7.20D-01

TightC=F SS= 1.41D+00 RLast= 3.34D-02 DXNew= 1.4142D-01 1.0019D-01

Trust test= 7.20D-01 RLast= 3.34D-02 DXMaxT set to 1.00D-01

ITU= 1 0 0 1 -1 -1 1 1 -1 1 1 1 -1 0 1 -1 1 1 1 1

ITU= 0 0

Eigenvalues --- 0.00020 0.00878 0.00878 0.00878 0.00878

Eigenvalues --- 0.01337 0.01339 0.01347 0.01348 0.01603

Eigenvalues --- 0.01623 0.01631 0.01640 0.01774 0.01793

Eigenvalues --- 0.01810 0.01823 0.01890 0.01909 0.01939

Eigenvalues --- 0.01950 0.01997 0.02000 0.02045 0.02047

Eigenvalues --- 0.02070 0.02087 0.02103 0.02111 0.02115

Eigenvalues --- 0.02205 0.02313 0.02316 0.02351 0.02373

Eigenvalues --- 0.07187 0.07187 0.07192 0.07192 0.07202

Eigenvalues --- 0.07313 0.07382 0.07390 0.10696 0.13290

Eigenvalues --- 0.14206 0.14498 0.14499 0.15544 0.15821

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16009 0.16133 0.16345 0.16630 0.18126

Eigenvalues --- 0.22063 0.22090 0.22094 0.23232 0.23841

Eigenvalues --- 0.23853 0.24038 0.24810 0.24977 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25532 0.26822 0.29214 0.30826 0.32817

Eigenvalues --- 0.33189 0.33197 0.33282 0.33282 0.33335

Eigenvalues --- 0.33586 0.33704 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33724 0.33724 0.34112 0.34430

Eigenvalues --- 0.34437 0.34437 0.34464 0.34842 0.35555

Eigenvalues --- 0.35564 0.35653 0.35682 0.35682 0.35986

Eigenvalues --- 0.38406 0.39185 0.41644 0.41819 0.45324

Eigenvalues --- 0.46104 0.46628 0.48969 0.48982 0.51077

Eigenvalues --- 0.51358 0.51361 0.53404 0.54005 0.54017

Eigenvalues --- 0.54024 0.56321 0.56330 0.56351

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 0.73205 0.26795

Cosine: 1.000 > 0.970

Length: 0.999

GDIIS step was calculated using 2 of the last 22 vectors.

Maximum step size ( 0.100) exceeded in Quadratic search.

-- Step size scaled by 0.079

Iteration 1 RMS(Cart)= 0.01127023 RMS(Int)= 0.00005403

Iteration 2 RMS(Cart)= 0.00011052 RMS(Int)= 0.00000883

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000883

ITry= 1 IFail=0 DXMaxC= 5.12D-02 DCOld= 1.00D+10 DXMaxT= 1.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.11D-09 for atom 29.

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

(Linear) (Quad) (Total)

R1 2.58172 0.00009 -0.00016 0.01252 0.01239 2.59411

R2 2.73374 -0.00045 0.00006 -0.02590 -0.02582 2.70792

R3 2.58633 0.00001 0.00003 0.00353 0.00355 2.58988

R4 2.56151 0.00009 0.00018 -0.01052 -0.01035 2.55116

R5 3.80035 -0.00004 -0.00008 0.01064 0.01060 3.81094

R6 2.77683 -0.00074 -0.00012 -0.02110 -0.02124 2.75559

R7 2.57956 0.00018 -0.00006 0.01495 0.01487 2.59443

R8 2.59660 0.00043 0.00004 0.01753 0.01756 2.61415

R9 2.81319 -0.00010 0.00001 -0.00175 -0.00174 2.81145

R10 2.04328 -0.00004 0.00001 0.00013 0.00014 2.04342

R11 2.49705 0.00017 -0.00004 -0.00518 -0.00525 2.49180

R12 2.58263 0.00005 0.00013 -0.00979 -0.00966 2.57297

R13 2.80082 -0.00006 -0.00009 0.00549 0.00540 2.80622

R14 2.57704 0.00025 -0.00011 0.01493 0.01481 2.59185

R15 3.78441 -0.00012 -0.00008 0.00789 0.00784 3.79224

R16 2.84259 -0.00035 -0.00003 -0.01168 -0.01172 2.83087

R17 2.48783 -0.00001 0.00006 -0.01758 -0.01754 2.47029

R18 2.54971 0.00019 0.00006 0.00172 0.00177 2.55148

R19 2.80686 0.00000 0.00003 0.00198 0.00201 2.80887

R20 2.04347 -0.00009 -0.00001 -0.00214 -0.00215 2.04132

R21 2.48783 -0.00001 0.00006 -0.01758 -0.01754 2.47029

R22 2.54971 0.00019 0.00006 0.00172 0.00177 2.55148

R23 2.84259 -0.00035 -0.00003 -0.01168 -0.01172 2.83087

R24 2.80686 0.00000 0.00003 0.00198 0.00201 2.80887

R25 2.80082 -0.00006 -0.00009 0.00549 0.00540 2.80622

R26 2.04347 -0.00009 -0.00001 -0.00214 -0.00215 2.04132

R27 2.58263 0.00005 0.00013 -0.00979 -0.00966 2.57297

R28 2.49705 0.00017 -0.00004 -0.00518 -0.00525 2.49180

R29 2.57704 0.00025 -0.00011 0.01493 0.01481 2.59185

R30 3.78441 -0.00012 -0.00008 0.00789 0.00784 3.79224

R31 2.57956 0.00018 -0.00006 0.01495 0.01487 2.59443

R32 2.56151 0.00009 0.00018 -0.01052 -0.01035 2.55116

R33 2.58172 0.00009 -0.00016 0.01252 0.01239 2.59411

R34 3.80035 -0.00004 -0.00008 0.01064 0.01060 3.81094

R35 2.77683 -0.00074 -0.00012 -0.02110 -0.02124 2.75559

R36 2.59660 0.00043 0.00004 0.01753 0.01756 2.61415

R37 2.81319 -0.00010 0.00001 -0.00175 -0.00174 2.81145

R38 2.73374 -0.00045 0.00006 -0.02590 -0.02582 2.70792

R39 2.04328 -0.00004 0.00001 0.00013 0.00014 2.04342

R40 2.58633 0.00001 0.00003 0.00353 0.00355 2.58988

R41 2.06250 -0.00004 0.00000 -0.00029 -0.00028 2.06222

R42 2.06973 -0.00006 0.00001 -0.00077 -0.00076 2.06897

R43 2.06973 -0.00006 0.00001 -0.00077 -0.00076 2.06897

R44 2.06897 -0.00006 0.00002 -0.00131 -0.00128 2.06769

R45 2.06897 -0.00006 0.00002 -0.00131 -0.00128 2.06769

R46 2.06172 -0.00004 0.00001 -0.00045 -0.00045 2.06128

R47 2.06897 -0.00006 0.00002 -0.00131 -0.00128 2.06769

R48 2.06897 -0.00006 0.00002 -0.00131 -0.00128 2.06769

R49 2.06172 -0.00004 0.00001 -0.00045 -0.00045 2.06128

R50 2.06973 -0.00006 0.00001 -0.00077 -0.00076 2.06897

R51 2.06973 -0.00006 0.00001 -0.00077 -0.00076 2.06897

R52 2.06250 -0.00004 0.00000 -0.00029 -0.00028 2.06222

A1 1.89133 0.00010 0.00005 0.00027 0.00034 1.89167

A2 2.20379 0.00024 0.00006 0.00023 0.00030 2.20409

A3 2.18806 -0.00034 -0.00011 -0.00049 -0.00064 2.18743

A4 1.90795 0.00001 -0.00004 0.00280 0.00273 1.91068

A5 2.19260 -0.00010 0.00003 -0.01474 -0.01468 2.17792

A6 2.18263 0.00009 0.00001 0.01194 0.01195 2.19458

A7 1.89504 -0.00013 0.00001 -0.00370 -0.00369 1.89135

A8 2.22459 -0.00005 -0.00007 -0.00542 -0.00549 2.21911

A9 2.16355 0.00018 0.00007 0.00912 0.00918 2.17273

A10 1.85085 0.00031 0.00002 0.00697 0.00698 1.85783

A11 2.17216 0.00005 0.00009 0.00515 0.00524 2.17740

A12 2.26018 -0.00036 -0.00011 -0.01212 -0.01222 2.24796

A13 1.87960 -0.00028 -0.00004 -0.00634 -0.00636 1.87324

A14 2.17982 0.00017 0.00004 0.00870 0.00874 2.18856

A15 2.22376 0.00011 -0.00000 -0.00237 -0.00238 2.22138

A16 2.16922 -0.00011 0.00007 -0.00683 -0.00679 2.16244

A17 2.23115 0.00001 -0.00004 0.00570 0.00566 2.23681

A18 2.16837 0.00013 0.00005 0.00204 0.00208 2.17045

A19 1.88366 -0.00014 -0.00001 -0.00774 -0.00774 1.87592

A20 1.91538 -0.00008 -0.00003 0.00536 0.00532 1.92070

A21 2.18796 0.00008 -0.00001 0.00673 0.00674 2.19470

A22 2.17984 -0.00000 0.00003 -0.01209 -0.01206 2.16778

A23 1.88315 0.00019 0.00006 -0.00223 -0.00216 1.88099

A24 2.24653 0.00009 0.00003 0.00105 0.00107 2.24760

A25 2.15351 -0.00028 -0.00009 0.00118 0.00109 2.15460

A26 1.85734 -0.00020 -0.00003 -0.00138 -0.00142 1.85592

A27 2.15273 0.00027 0.00006 0.00756 0.00762 2.16034

A28 2.27312 -0.00008 -0.00002 -0.00618 -0.00620 2.26693

A29 1.88526 0.00022 0.00002 0.00599 0.00600 1.89126

A30 2.16461 -0.00005 0.00002 0.00094 0.00096 2.16557

A31 2.23332 -0.00017 -0.00003 -0.00693 -0.00695 2.22636

A32 2.17282 -0.00025 -0.00012 0.01343 0.01330 2.18612

A33 1.85734 -0.00020 -0.00003 -0.00138 -0.00142 1.85592

A34 2.27312 -0.00008 -0.00002 -0.00618 -0.00620 2.26693

A35 2.15273 0.00027 0.00006 0.00756 0.00762 2.16034

A36 1.88526 0.00022 0.00002 0.00599 0.00600 1.89126

A37 2.23332 -0.00017 -0.00003 -0.00693 -0.00695 2.22636

A38 2.16461 -0.00005 0.00002 0.00094 0.00096 2.16557

A39 1.88366 -0.00014 -0.00001 -0.00774 -0.00774 1.87592

A40 2.16837 0.00013 0.00005 0.00204 0.00208 2.17045

A41 2.23115 0.00001 -0.00004 0.00570 0.00566 2.23681

A42 1.91538 -0.00008 -0.00003 0.00536 0.00532 1.92070

A43 2.18796 0.00008 -0.00001 0.00673 0.00674 2.19470

A44 2.17984 -0.00000 0.00003 -0.01209 -0.01206 2.16778

A45 2.15351 -0.00028 -0.00009 0.00118 0.00109 2.15460

A46 2.24653 0.00009 0.00003 0.00105 0.00107 2.24760

A47 1.88315 0.00019 0.00006 -0.00223 -0.00216 1.88099

A48 2.16922 -0.00011 0.00007 -0.00683 -0.00679 2.16244

A49 1.90795 0.00001 -0.00004 0.00280 0.00273 1.91068

A50 2.18263 0.00009 0.00001 0.01194 0.01195 2.19458

A51 2.19260 -0.00010 0.00003 -0.01474 -0.01468 2.17792

A52 2.22459 -0.00005 -0.00007 -0.00542 -0.00549 2.21911

A53 2.16355 0.00018 0.00007 0.00912 0.00918 2.17273

A54 1.89504 -0.00013 0.00001 -0.00370 -0.00369 1.89135

A55 1.85085 0.00031 0.00002 0.00697 0.00698 1.85783

A56 2.17216 0.00005 0.00009 0.00515 0.00524 2.17740

A57 2.26018 -0.00036 -0.00011 -0.01212 -0.01222 2.24796

A58 1.87960 -0.00028 -0.00004 -0.00634 -0.00636 1.87324

A59 2.22376 0.00011 -0.00000 -0.00237 -0.00238 2.22138

A60 2.17982 0.00017 0.00004 0.00870 0.00874 2.18856

A61 1.89133 0.00010 0.00005 0.00027 0.00034 1.89167

A62 2.20379 0.00024 0.00006 0.00023 0.00030 2.20409

A63 2.18806 -0.00034 -0.00011 -0.00049 -0.00064 2.18743

A64 2.17282 -0.00025 -0.00012 0.01343 0.01330 2.18612

A65 1.57080 -0.00003 0.00003 -0.01212 -0.01208 1.55873

A66 1.57079 0.00003 -0.00003 0.01212 0.01208 1.58287

A67 1.57079 0.00003 -0.00003 0.01212 0.01208 1.58287

A68 1.57080 -0.00003 0.00003 -0.01212 -0.01208 1.55873

A69 1.94401 -0.00010 -0.00004 -0.00636 -0.00641 1.93759

A70 1.94063 -0.00003 -0.00001 -0.00089 -0.00090 1.93973

A71 1.94063 -0.00003 -0.00001 -0.00089 -0.00090 1.93973

A72 1.88930 0.00005 0.00000 0.00057 0.00056 1.88986

A73 1.88930 0.00005 0.00000 0.00057 0.00056 1.88986

A74 1.85672 0.00007 0.00005 0.00769 0.00774 1.86446

A75 1.93408 -0.00003 0.00000 -0.00158 -0.00158 1.93250

A76 1.93408 -0.00003 0.00000 -0.00158 -0.00158 1.93250

A77 1.94588 -0.00006 -0.00001 -0.00689 -0.00691 1.93897

A78 1.85720 0.00005 0.00001 0.00818 0.00820 1.86539

A79 1.89489 0.00004 -0.00001 0.00133 0.00131 1.89620

A80 1.89489 0.00004 -0.00001 0.00133 0.00131 1.89620

A81 1.93408 -0.00003 0.00000 -0.00158 -0.00158 1.93250

A82 1.93408 -0.00003 0.00000 -0.00158 -0.00158 1.93250

A83 1.94588 -0.00006 -0.00001 -0.00689 -0.00691 1.93897

A84 1.85720 0.00005 0.00001 0.00818 0.00820 1.86539

A85 1.89489 0.00004 -0.00001 0.00133 0.00131 1.89620

A86 1.89489 0.00004 -0.00001 0.00133 0.00131 1.89620

A87 1.94063 -0.00003 -0.00001 -0.00089 -0.00090 1.93973

A88 1.94063 -0.00003 -0.00001 -0.00089 -0.00090 1.93973

A89 1.94401 -0.00010 -0.00004 -0.00636 -0.00641 1.93759

A90 1.85672 0.00007 0.00005 0.00769 0.00774 1.86446

A91 1.88930 0.00005 0.00000 0.00057 0.00056 1.88986

A92 1.88930 0.00005 0.00000 0.00057 0.00056 1.88986

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 1.03273 0.00003 0.00003 0.00424 0.00427 1.03699

D31 -1.03273 -0.00003 -0.00003 -0.00424 -0.00427 -1.03699

D32 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.10887 0.00003 0.00003 0.00424 0.00427 -2.10460

D34 2.10887 -0.00003 -0.00003 -0.00424 -0.00427 2.10460

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 1.02883 0.00001 0.00001 0.00409 0.00409 1.03292

D64 -1.02883 -0.00001 -0.00001 -0.00409 -0.00409 -1.03292

D65 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D66 -2.11277 0.00001 0.00001 0.00409 0.00409 -2.10867

D67 2.11277 -0.00001 -0.00001 -0.00409 -0.00409 2.10867

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 -2.11277 0.00001 0.00001 0.00409 0.00409 -2.10867

D80 2.11277 -0.00001 -0.00001 -0.00409 -0.00409 2.10867

D81 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D82 1.02883 0.00001 0.00001 0.00409 0.00409 1.03292

D83 -1.02883 -0.00001 -0.00001 -0.00409 -0.00409 -1.03292

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

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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 1.03273 0.00003 0.00003 0.00424 0.00427 1.03699

D126 -1.03273 -0.00003 -0.00003 -0.00424 -0.00427 -1.03699

D127 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D128 -2.10887 0.00003 0.00003 0.00424 0.00427 -2.10460

D129 2.10887 -0.00003 -0.00003 -0.00424 -0.00427 2.10460

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 0.000738 0.000450 NO

RMS Force 0.000129 0.000300 YES

Maximum Displacement 0.051173 0.001800 NO

RMS Displacement 0.011270 0.001200 NO

Predicted change in Energy=-1.308162D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:27:53 2019, MaxMem= 2415919104 cpu: 1.3

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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1 6 0 -2.070161 -2.196481 0.000000

2 7 0 -0.734872 -1.878004 0.000000

3 6 0 -0.001795 -3.011646 0.000000

4 6 0 -0.914406 -4.148956 0.000000

5 6 0 -2.194306 -3.624060 0.000000

6 7 0 1.367330 -3.113545 0.000000

7 6 0 2.181951 -2.076669 0.000000

8 7 0 1.859826 -0.753768 0.000000

9 6 0 3.000452 0.007887 0.000000

10 6 0 4.172918 -0.924540 0.000000

11 6 0 3.663678 -2.175008 0.000000

12 7 0 -3.115399 -1.310045 0.000000

13 6 0 -4.172918 0.924540 0.000000

14 6 0 -3.663678 2.175008 0.000000

15 6 0 -2.181951 2.076669 0.000000

16 7 0 -1.859826 0.753768 0.000000

17 6 0 -3.000452 -0.007887 0.000000

18 7 0 -1.367330 3.113545 0.000000

19 7 0 0.734872 1.878004 0.000000

20 6 0 0.001795 3.011646 0.000000

21 6 0 0.914406 4.148956 0.000000

22 6 0 2.194306 3.624060 0.000000

23 6 0 2.070161 2.196481 0.000000

24 7 0 3.115399 1.310045 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.491870 -5.575449 0.000000

27 1 0 -3.126728 -4.171665 0.000000

28 6 0 5.588730 -0.471956 0.000000

29 1 0 4.208365 -3.107848 0.000000

30 6 0 -5.588730 0.471956 0.000000

31 1 0 -4.208365 3.107848 0.000000

32 6 0 0.491870 5.575449 0.000000

33 1 0 3.126728 4.171665 0.000000

34 1 0 -1.357460 -6.240012 0.000000

35 1 0 0.118458 -5.806447 0.879113

36 1 0 0.118458 -5.806447 -0.879113

37 1 0 5.797901 0.145333 0.878872

38 1 0 5.797901 0.145333 -0.878872

39 1 0 6.272548 -1.321779 0.000000

40 1 0 -5.797901 -0.145333 0.878872

41 1 0 -5.797901 -0.145333 -0.878872

42 1 0 -6.272548 1.321779 0.000000

43 1 0 -0.118458 5.806447 0.879113

44 1 0 -0.118458 5.806447 -0.879113

45 1 0 1.357460 6.240012 0.000000

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Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.372743 0.000000

3 C 2.223204 1.350018 0.000000

4 C 2.268905 2.278038 1.458195 0.000000

5 C 1.432967 2.275667 2.276435 1.383351 0.000000

6 N 3.557718 2.438405 1.372912 2.505673 3.598038

7 C 4.253800 2.923581 2.375485 3.725829 4.641772

8 N 4.186433 2.827785 2.926371 4.384480 4.967350

9 C 5.529047 4.184404 4.258059 5.710119 6.338498

10 C 6.371332 4.999549 4.667359 6.023099 6.915848

11 C 5.733879 4.408566 3.759741 4.985511 6.034544

12 N 1.370508 2.447343 3.548237 3.592185 2.490598

13 C 3.763291 4.435585 5.735140 6.029782 4.960309

14 C 4.652871 5.000481 6.349077 6.895725 5.982328

15 C 4.274611 4.211113 5.535705 6.353352 5.700742

16 N 2.957736 2.862122 4.198884 4.993047 4.390587

17 C 2.378105 2.937719 4.244351 4.636814 3.704940

18 N 5.356337 5.031457 6.275560 7.276610 6.788167

19 N 4.946679 4.033329 4.944831 6.248549 6.233201

20 C 5.605139 4.944831 6.023293 7.218978 6.989668

21 C 7.012290 6.248549 7.218978 8.497052 8.371611

22 C 7.215565 6.233201 6.989668 8.371611 8.473203

23 C 6.036586 4.946679 5.605139 7.012290 7.215565

24 N 6.259853 4.998824 5.328594 6.785279 7.248335

25 Zn 3.018293 2.016664 3.011647 4.248526 4.236601

26 C 3.729401 3.705422 2.610222 1.487756 2.589634

27 H 2.240020 3.313889 3.333295 2.212439 1.081334

28 C 7.850643 6.478033 6.140357 7.470683 8.397107

29 H 6.344326 5.093928 4.211258 5.227493 6.423447

30 C 4.415980 5.392796 6.584021 6.572833 5.319724

31 H 5.719074 6.076501 7.425863 7.969402 7.026736

32 C 8.183330 7.553731 8.601274 9.825562 9.583659

33 H 8.219546 7.177078 7.835025 9.250054 9.438577

34 H 4.105860 4.406215 3.501453 2.137478 2.746546

35 H 4.312163 4.115055 2.932271 2.141711 3.299171

36 H 4.312163 4.115055 2.932271 2.141711 3.299171

37 H 8.256083 6.895174 6.661486 8.016757 8.880096

38 H 8.256083 6.895174 6.661486 8.016757 8.880096

39 H 8.388438 7.029461 6.497925 7.723033 8.774287

40 H 4.344614 5.422990 6.525566 6.375730 5.085259

41 H 4.344614 5.422990 6.525566 6.375730 5.085259

42 H 5.480712 6.395660 7.622396 7.657587 6.410412

43 H 8.284253 7.759098 8.862574 10.025788 9.696208

44 H 8.284253 7.759098 8.862574 10.025788 9.696208

45 H 9.106206 8.383319 9.350976 10.634473 10.484033

6 7 8 9 10

6 N 0.000000

7 C 1.318605 0.000000

8 N 2.410623 1.361555 0.000000

9 C 3.522843 2.239490 1.371549 0.000000

10 C 3.558520 2.300293 2.319387 1.498031 0.000000

11 C 2.480738 1.484986 2.296477 2.281425 1.350184

12 N 4.831923 5.352535 5.006228 6.256244 7.298506

13 C 6.855690 7.027917 6.261846 7.231701 8.548221

14 C 7.299304 7.228287 6.251946 7.007642 8.427303

15 C 6.287743 6.024438 4.934302 5.580069 7.027917

16 N 5.036928 4.934302 4.013537 4.917179 6.261846

17 C 5.359350 5.580069 4.917179 6.000926 7.231701

18 N 6.801104 6.287743 5.036928 5.359350 6.855690

19 N 5.031457 4.211113 2.862122 2.937719 4.435585

20 C 6.275560 5.535705 4.198884 4.244351 5.735140

21 C 7.276610 6.353352 4.993047 4.636814 6.029782

22 C 6.788167 5.700742 4.390587 3.704940 4.960309

23 C 5.356337 4.274611 2.957736 2.378105 3.763291

24 N 4.756458 3.512998 2.415737 1.307221 2.472188

25 Zn 3.400552 3.012219 2.006768 3.000463 4.274110

26 C 3.085061 4.403497 5.364615 6.585587 6.587200

27 H 4.616945 5.707108 6.045473 7.416940 7.989284

28 C 4.979780 3.765799 3.739537 2.632381 1.486390

29 H 2.841040 2.273693 3.325256 3.341684 2.183595

30 C 7.825765 8.177957 7.548734 8.601710 9.861033

31 H 8.354286 8.228934 7.192706 7.847089 9.300863

32 C 8.732986 7.836535 6.475360 6.106614 7.469938

33 H 7.494649 6.319358 5.085757 4.165692 5.202482

34 H 4.147201 5.464509 6.360016 7.617588 7.670679

35 H 3.095844 4.352252 5.416159 6.548681 6.406599

36 H 3.095844 4.352252 5.416159 6.548681 6.406599

37 H 5.569798 4.334143 4.133912 2.935477 2.134857

38 H 5.569798 4.334143 4.133912 2.935477 2.134857

39 H 5.222220 4.159668 4.449129 3.531943 2.136878

40 H 7.805334 8.257149 7.731972 8.843467 10.039761

41 H 7.805334 8.257149 7.731972 8.843467 10.039761

42 H 8.834016 9.111971 8.393057 9.365621 10.684274

43 H 9.085520 8.258828 6.908174 6.642570 8.030874

44 H 9.085520 8.258828 6.908174 6.642570 8.030874

45 H 9.353562 8.357449 7.011799 6.445060 7.697896

11 12 13 14 15

11 C 0.000000

12 N 6.834036 0.000000

13 C 8.427303 2.472188 0.000000

14 C 8.521314 3.527918 1.350184 0.000000

15 C 7.228287 3.512998 2.300293 1.484986 0.000000

16 N 6.251946 2.415737 2.319387 2.296477 1.361555

17 C 7.007642 1.307221 1.498031 2.281425 2.239490

18 N 7.299304 4.756458 3.558520 2.480738 1.318605

19 N 5.000481 4.998824 4.999549 4.408566 2.923581

20 C 6.349077 5.328594 4.667359 3.759741 2.375485

21 C 6.895725 6.785279 6.023099 4.985511 3.725829

22 C 5.982328 7.248335 6.915848 6.034544 4.641772

23 C 4.652871 6.259853 6.371332 5.733879 4.253800

24 N 3.527918 6.759269 7.298506 6.834036 5.352535

25 Zn 4.260657 3.379635 4.274110 4.260657 3.012219

26 C 5.369504 5.007652 7.469938 8.374363 7.836535

27 H 7.077871 2.861643 5.202482 6.369347 6.319358

28 C 2.570255 8.744385 9.861033 9.623590 8.177957

29 H 1.080219 7.541195 9.300863 9.480381 8.228934

30 C 9.623590 3.048424 1.486390 2.570255 3.765799

31 H 9.480381 4.551082 2.183595 1.080219 2.273693

32 C 8.374363 7.773186 6.587200 5.369504 4.403497

33 H 6.369347 8.307424 7.989284 7.077871 5.707108

34 H 6.460347 5.234016 7.697896 8.725320 8.357449

35 H 5.150609 5.607879 8.030874 8.875868 8.258828

36 H 5.150609 5.607879 8.030874 8.875868 8.258828

37 H 3.272813 9.073999 10.039761 9.716659 8.257149

38 H 3.272813 9.073999 10.039761 9.716659 8.257149

39 H 2.744850 9.387955 10.684274 10.533571 9.111971

40 H 9.716659 3.053651 2.134857 3.272813 4.334143

41 H 9.716659 3.053651 2.134857 3.272813 4.334143

42 H 10.533571 4.110241 2.136878 2.744850 4.159668

43 H 8.875868 7.771677 6.406599 5.150609 4.352252

44 H 8.875868 7.771677 6.406599 5.150609 4.352252

45 H 8.725320 8.775524 7.670679 6.460347 5.464509

16 17 18 19 20

16 N 0.000000

17 C 1.371549 0.000000

18 N 2.410623 3.522843 0.000000

19 N 2.827785 4.184404 2.438405 0.000000

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21 C 4.384480 5.710119 2.505673 2.278038 1.458195

22 C 4.967350 6.338498 3.598038 2.275667 2.276435

23 C 4.186433 5.529047 3.557718 1.372743 2.223204

24 N 5.006228 6.256244 4.831923 2.447343 3.548237

25 Zn 2.006768 3.000463 3.400552 2.016664 3.011647

26 C 6.475360 6.106614 8.732986 7.553731 8.601274

27 H 5.085757 4.165692 7.494649 7.177078 7.835025

28 C 7.548734 8.601710 7.825765 5.392796 6.584021

29 H 7.192706 7.847089 8.354286 6.076501 7.425863

30 C 3.739537 2.632381 4.979780 6.478033 6.140357

31 H 3.325256 3.341684 2.841040 5.093928 4.211258

32 C 5.364615 6.585587 3.085061 3.705422 2.610222

33 H 6.045473 7.416940 4.616945 3.313889 3.333295

34 H 7.011799 6.445060 9.353562 8.383319 9.350976

35 H 6.908174 6.642570 9.085520 7.759098 8.862574

36 H 6.908174 6.642570 9.085520 7.759098 8.862574

37 H 7.731972 8.843467 7.805334 5.422990 6.525566

38 H 7.731972 8.843467 7.805334 5.422990 6.525566

39 H 8.393057 9.365621 8.834016 6.395660 7.622396

40 H 4.133912 2.935477 5.569798 6.895174 6.661486

41 H 4.133912 2.935477 5.569798 6.895174 6.661486

42 H 4.449129 3.531943 5.222220 7.029461 6.497925

43 H 5.416159 6.548681 3.095844 4.115055 2.932271

44 H 5.416159 6.548681 3.095844 4.115055 2.932271

45 H 6.360016 7.617588 4.147201 4.406215 3.501453

21 22 23 24 25

21 C 0.000000

22 C 1.383351 0.000000

23 C 2.268905 1.432967 0.000000

24 N 3.592185 2.490598 1.370508 0.000000

25 Zn 4.248526 4.236601 3.018293 3.379635 0.000000

26 C 9.825562 9.583659 8.183330 7.773186 5.597104

27 H 9.250054 9.438577 8.219546 8.307424 5.213369

28 C 6.572833 5.319724 4.415980 3.048424 5.608622

29 H 7.969402 7.026736 5.719074 4.551082 5.231544

30 C 7.470683 8.397107 7.850643 8.744385 5.608622

31 H 5.227493 6.423447 6.344326 7.541195 5.231544

32 C 1.487756 2.589634 3.729401 5.007652 5.597104

33 H 2.212439 1.081334 2.240020 2.861643 5.213369

34 H 10.634473 10.484033 9.106206 8.775524 6.385957

35 H 10.025788 9.696208 8.284253 7.771677 5.873815

36 H 10.025788 9.696208 8.284253 7.771677 5.873815

37 H 6.375730 5.085259 4.344614 3.053651 5.865935

38 H 6.375730 5.085259 4.344614 3.053651 5.865935

39 H 7.657587 6.410412 5.480712 4.110241 6.410301

40 H 8.016757 8.880096 8.256083 9.073999 5.865935

41 H 8.016757 8.880096 8.256083 9.073999 5.865935

42 H 7.723033 8.774287 8.388438 9.387955 6.410301

43 H 2.141711 3.299171 4.312163 5.607879 5.873815

44 H 2.141711 3.299171 4.312163 5.607879 5.873815

45 H 2.137478 2.746546 4.105860 5.234016 6.385957

26 27 28 29 30

26 C 0.000000

27 H 2.985479 0.000000

28 C 7.938472 9.468213 0.000000

29 H 5.308603 7.411835 2.975455 0.000000

30 C 7.908798 5.255918 11.217245 10.430631 0.000000

31 H 9.445209 7.359432 10.430631 10.463088 2.975455

32 C 11.194207 10.397139 7.908798 9.445209 7.938472

33 H 10.397139 10.426738 5.255918 7.359432 9.468213

34 H 1.091279 2.721831 9.028844 6.386616 7.934366

35 H 1.094852 3.738527 7.691132 4.978215 8.530134

36 H 1.094852 3.738527 7.691132 4.978215 8.530134

37 H 8.547572 9.952783 1.094172 3.725885 11.425168

38 H 8.547572 9.952783 1.094172 3.725885 11.425168

39 H 7.990686 9.821825 1.090782 2.729632 11.996141

40 H 7.642810 4.911103 11.425168 10.472548 1.094172

41 H 7.642810 4.911103 11.425168 10.472548 1.094172

42 H 8.999333 6.330412 11.996141 11.378538 1.090782

43 H 11.421902 10.458741 8.530134 9.947808 7.691132

44 H 11.421902 10.458741 8.530134 9.947808 7.691132

45 H 11.959312 11.336267 7.934366 9.772929 9.028844

31 32 33 34 35

31 H 0.000000

32 C 5.308603 0.000000

33 H 7.411835 2.985479 0.000000

34 H 9.772929 11.959312 11.336267 0.000000

35 H 9.947808 11.421902 10.458741 1.771765 0.000000

36 H 9.947808 11.421902 10.458741 1.771765 1.758227

37 H 10.472548 7.642810 4.911103 9.630380 8.226771

38 H 10.472548 7.642810 4.911103 9.630380 8.412507

39 H 11.378538 8.999333 6.330412 9.077777 7.665371

40 H 3.725885 8.547572 9.952783 7.591775 8.188499

41 H 3.725885 8.547572 9.952783 7.591775 8.375084

42 H 2.729632 7.990686 9.821825 9.018801 9.614021

43 H 4.978215 1.094852 3.738527 12.141876 11.615311

44 H 4.978215 1.094852 3.738527 12.141876 11.747630

45 H 6.386616 1.091279 2.721831 12.771914 12.141876

36 37 38 39 40

36 H 0.000000

37 H 8.412507 0.000000

38 H 8.226771 1.757743 0.000000

39 H 7.665371 1.774858 1.774858 0.000000

40 H 8.375084 11.599444 11.731870 12.159448 0.000000

41 H 8.188499 11.731870 11.599444 12.159448 1.757743

42 H 9.614021 12.159448 12.159448 12.820602 1.774858

43 H 11.747630 8.188499 8.375084 9.614021 8.226771

44 H 11.615311 8.375084 8.188499 9.614021 8.412507

45 H 12.141876 7.591775 7.591775 9.018801 9.630380

41 42 43 44 45

41 H 0.000000

42 H 1.774858 0.000000

43 H 8.412507 7.665371 0.000000

44 H 8.226771 7.665371 1.758227 0.000000

45 H 9.630380 9.077777 1.771765 1.771765 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=0 Diff= 5.61D-03

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 2.813226 -1.093551 0.000000

2 7 0 2.016517 0.024340 0.000000

3 6 0 2.791798 1.129549 0.000000

4 6 0 4.188618 0.710950 0.000000

5 6 0 4.182904 -0.672389 0.000000

6 7 0 2.371974 2.436697 0.000000

7 6 0 1.105040 2.802205 0.000000

8 7 0 0.000000 2.006768 0.000000

9 6 0 -1.134317 2.777787 0.000000

10 6 0 -0.710558 4.214632 0.000000

11 6 0 0.639624 4.212372 0.000000

12 7 0 2.384302 -2.395210 0.000000

13 6 0 0.710558 -4.214632 0.000000

14 6 0 -0.639624 -4.212372 0.000000

15 6 0 -1.105040 -2.802205 0.000000

16 7 0 -0.000000 -2.006768 0.000000

17 6 0 1.134317 -2.777787 0.000000

18 7 0 -2.371974 -2.436697 0.000000

19 7 0 -2.016517 -0.024340 0.000000

20 6 0 -2.791798 -1.129549 0.000000

21 6 0 -4.188618 -0.710950 0.000000

22 6 0 -4.182904 0.672389 0.000000

23 6 0 -2.813226 1.093551 0.000000

24 7 0 -2.384302 2.395210 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 5.351949 1.638355 0.000000

27 1 0 5.040641 -1.330849 0.000000

28 6 0 -1.661799 5.356778 0.000000

29 1 0 1.299566 5.067561 0.000000

30 6 0 1.661799 -5.356778 0.000000

31 1 0 -1.299566 -5.067561 0.000000

32 6 0 -5.351949 -1.638355 0.000000

33 1 0 -5.040641 1.330849 0.000000

34 1 0 6.292977 1.085765 0.000000

35 1 0 5.336786 2.290759 0.879113

36 1 0 5.336786 2.290759 -0.879113

37 1 0 -2.312456 5.318771 0.878872

38 1 0 -2.312456 5.318771 -0.878872

39 1 0 -1.131054 6.309729 0.000000

40 1 0 2.312456 -5.318771 0.878872

41 1 0 2.312456 -5.318771 -0.878872

42 1 0 1.131054 -6.309729 0.000000

43 1 0 -5.336786 -2.290759 0.879113

44 1 0 -5.336786 -2.290759 -0.879113

45 1 0 -6.292977 -1.085765 0.000000

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

Rotational constants (GHZ): 0.1828901 0.1817132 0.0913552

Leave Link 202 at Tue Sep 17 14:27:53 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 101 beta electrons

nuclear repulsion energy 2761.1246794727 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= -0.1142495641 Hartrees.

Nuclear repulsion after empirical dispersion term = 2761.0104299085 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 = 3504

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.59D-08

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 140

GePol: Fraction of low-weight points (<1% of avg) = 4.00%

GePol: Cavity surface area = 382.066 Ang\*\*2

GePol: Cavity volume = 379.246 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0106940439 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2760.9997358646 Hartrees.

Leave Link 301 at Tue Sep 17 14:27:53 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= 15319 LenP2D= 41250.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.83D-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 14:27:54 2019, MaxMem= 2415919104 cpu: 12.5

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:27:54 2019, MaxMem= 2415919104 cpu: 1.2

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= 0.000000 0.000000 -0.000000

Rot= 0.999997 0.000000 -0.000000 -0.002323 Ang= -0.27 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 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0178 S= 1.0059

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= -1276.14904717454

Leave Link 401 at Tue Sep 17 14:27:56 2019, MaxMem= 2415919104 cpu: 38.4

(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= 36834048.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.22D-15 for 3504.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.55D-15 for 2542 1319.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.88D-15 for 3504.

Iteration 1 A^-1\*A deviation from orthogonality is 3.02D-12 for 2428 2387.

E= -1275.84037905144

DIIS: error= 9.31D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.84037905144 IErMin= 1 ErrMin= 9.31D-04

ErrMax= 9.31D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.51D-03 BMatP= 3.51D-03

IDIUse=3 WtCom= 9.91D-01 WtEn= 9.31D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.306 Goal= None Shift= 0.000

Gap= 0.392 Goal= None Shift= 0.000

RMSDP=9.22D-05 MaxDP=3.21D-03 OVMax= 1.96D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 9.22D-05 CP: 1.00D+00

E= -1275.84161033176 Delta-E= -0.001231280314 Rises=F Damp=F

DIIS: error= 4.28D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84161033176 IErMin= 2 ErrMin= 4.28D-04

ErrMax= 4.28D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.57D-04 BMatP= 3.51D-03

IDIUse=3 WtCom= 9.96D-01 WtEn= 4.28D-03

Coeff-Com: 0.696D-01 0.930D+00

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

Coeff: 0.693D-01 0.931D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=3.01D-05 MaxDP=1.23D-03 DE=-1.23D-03 OVMax= 1.58D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.95D-05 CP: 1.00D+00 1.07D+00

E= -1275.84159599878 Delta-E= 0.000014332977 Rises=F Damp=F

DIIS: error= 8.04D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1275.84161033176 IErMin= 2 ErrMin= 4.28D-04

ErrMax= 8.04D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.08D-04 BMatP= 2.57D-04

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

Coeff-Com: -0.179D-01 0.600D+00 0.417D+00

Coeff-En: 0.000D+00 0.544D+00 0.456D+00

Coeff: -0.466D-02 0.558D+00 0.446D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=1.99D-05 MaxDP=7.46D-04 DE= 1.43D-05 OVMax= 4.39D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.51D-05 CP: 1.00D+00 1.11D+00 5.84D-01

E= -1275.84170588985 Delta-E= -0.000109891065 Rises=F Damp=F

DIIS: error= 3.05D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84170588985 IErMin= 4 ErrMin= 3.05D-04

ErrMax= 3.05D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.48D-05 BMatP= 2.57D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.05D-03

Coeff-Com: -0.971D-02 0.150D+00 0.231D+00 0.629D+00

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

Coeff: -0.968D-02 0.150D+00 0.230D+00 0.630D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=9.96D-06 MaxDP=5.00D-04 DE=-1.10D-04 OVMax= 6.19D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 5.29D-06 CP: 1.00D+00 1.13D+00 8.62D-01 1.08D+00

E= -1275.84172358001 Delta-E= -0.000017690167 Rises=F Damp=F

DIIS: error= 1.64D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84172358001 IErMin= 5 ErrMin= 1.64D-04

ErrMax= 1.64D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.10D-06 BMatP= 3.48D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.64D-03

Coeff-Com: -0.234D-02-0.477D-02 0.586D-01 0.391D+00 0.558D+00

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

Coeff: -0.233D-02-0.477D-02 0.585D-01 0.390D+00 0.558D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=6.03D-06 MaxDP=2.50D-04 DE=-1.77D-05 OVMax= 3.87D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.20D-06 CP: 1.00D+00 1.15D+00 9.60D-01 1.37D+00 1.17D+00

E= -1275.84173188196 Delta-E= -0.000008301943 Rises=F Damp=F

DIIS: error= 1.09D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84173188196 IErMin= 6 ErrMin= 1.09D-04

ErrMax= 1.09D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.85D-06 BMatP= 9.10D-06

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.09D-03

Coeff-Com: 0.675D-02-0.105D+00-0.155D+00-0.227D+00 0.376D-01 0.144D+01

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

Coeff: 0.674D-02-0.105D+00-0.155D+00-0.227D+00 0.375D-01 0.144D+01

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=1.35D-05 MaxDP=6.66D-04 DE=-8.30D-06 OVMax= 9.51D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.27D-06 CP: 1.00D+00 1.18D+00 1.23D+00 1.93D+00 2.09D+00

CP: 2.13D+00

E= -1275.84174298935 Delta-E= -0.000011107393 Rises=F Damp=F

DIIS: error= 7.42D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84174298935 IErMin= 7 ErrMin= 7.42D-05

ErrMax= 7.42D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.02D-06 BMatP= 2.85D-06

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

Coeff-Com: 0.596D-02-0.694D-01-0.146D+00-0.341D+00-0.303D+00 0.108D+01

Coeff-Com: 0.774D+00

Coeff: 0.596D-02-0.694D-01-0.146D+00-0.341D+00-0.303D+00 0.108D+01

Coeff: 0.774D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=9.36D-06 MaxDP=4.29D-04 DE=-1.11D-05 OVMax= 6.57D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.45D-06 CP: 1.00D+00 1.21D+00 1.41D+00 2.32D+00 2.71D+00

CP: 3.00D+00 1.31D+00

E= -1275.84174694700 Delta-E= -0.000003957656 Rises=F Damp=F

DIIS: error= 2.86D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84174694700 IErMin= 8 ErrMin= 2.86D-05

ErrMax= 2.86D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.08D-07 BMatP= 2.02D-06

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

Coeff-Com: -0.341D-03 0.214D-01 0.617D-03-0.387D-01-0.161D+00-0.842D-01

Coeff-Com: 0.351D+00 0.911D+00

Coeff: -0.341D-03 0.214D-01 0.617D-03-0.387D-01-0.161D+00-0.842D-01

Coeff: 0.351D+00 0.911D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=4.10D-06 MaxDP=2.10D-04 DE=-3.96D-06 OVMax= 3.02D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.27D-06 CP: 1.00D+00 1.22D+00 1.48D+00 2.47D+00 3.00D+00

CP: 3.00D+00 1.77D+00 1.67D+00

E= -1275.84174769069 Delta-E= -0.000000743686 Rises=F Damp=F

DIIS: error= 1.33D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84174769069 IErMin= 9 ErrMin= 1.33D-05

ErrMax= 1.33D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.55D-07 BMatP= 4.08D-07

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

Coeff-Com: -0.153D-02 0.281D-01 0.330D-01 0.627D-01-0.658D-02-0.289D+00

Coeff-Com: -0.187D-01 0.493D+00 0.699D+00

Coeff: -0.153D-02 0.281D-01 0.330D-01 0.627D-01-0.658D-02-0.289D+00

Coeff: -0.187D-01 0.493D+00 0.699D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=1.24D-06 MaxDP=7.09D-05 DE=-7.44D-07 OVMax= 8.76D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 5.94D-07 CP: 1.00D+00 1.22D+00 1.50D+00 2.51D+00 3.00D+00

CP: 3.00D+00 1.96D+00 2.05D+00 1.22D+00

E= -1275.84174783776 Delta-E= -0.000000147066 Rises=F Damp=F

DIIS: error= 8.06D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84174783776 IErMin=10 ErrMin= 8.06D-06

ErrMax= 8.06D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.28D-08 BMatP= 1.55D-07

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

Coeff-Com: -0.704D-03 0.785D-02 0.160D-01 0.496D-01 0.544D-01-0.121D+00

Coeff-Com: -0.149D+00-0.274D-01 0.343D+00 0.827D+00

Coeff: -0.704D-03 0.785D-02 0.160D-01 0.496D-01 0.544D-01-0.121D+00

Coeff: -0.149D+00-0.274D-01 0.343D+00 0.827D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=7.60D-07 MaxDP=4.23D-05 DE=-1.47D-07 OVMax= 5.27D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 2.78D-07 CP: 1.00D+00 1.22D+00 1.51D+00 2.52D+00 3.00D+00

CP: 3.00D+00 2.08D+00 2.30D+00 1.44D+00 1.39D+00

E= -1275.84174789444 Delta-E= -0.000000056688 Rises=F Damp=F

DIIS: error= 4.74D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84174789444 IErMin=11 ErrMin= 4.74D-06

ErrMax= 4.74D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.49D-08 BMatP= 4.28D-08

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

Coeff-Com: 0.135D-03-0.516D-02-0.401D-02 0.570D-02 0.246D-01 0.342D-01

Coeff-Com: -0.741D-01-0.139D+00-0.751D-01 0.394D+00 0.839D+00

Coeff: 0.135D-03-0.516D-02-0.401D-02 0.570D-02 0.246D-01 0.342D-01

Coeff: -0.741D-01-0.139D+00-0.751D-01 0.394D+00 0.839D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=5.37D-07 MaxDP=3.18D-05 DE=-5.67D-08 OVMax= 3.87D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.35D-07 CP: 1.00D+00 1.22D+00 1.52D+00 2.54D+00 3.00D+00

CP: 3.00D+00 2.15D+00 2.45D+00 1.58D+00 1.73D+00

CP: 1.36D+00

E= -1275.84174791542 Delta-E= -0.000000020980 Rises=F Damp=F

DIIS: error= 2.18D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84174791542 IErMin=12 ErrMin= 2.18D-06

ErrMax= 2.18D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.40D-09 BMatP= 1.49D-08

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

Coeff-Com: 0.266D-03-0.491D-02-0.712D-02-0.100D-01-0.457D-02 0.540D-01

Coeff-Com: -0.498D-02-0.573D-01-0.153D+00-0.365D-01 0.452D+00 0.772D+00

Coeff: 0.266D-03-0.491D-02-0.712D-02-0.100D-01-0.457D-02 0.540D-01

Coeff: -0.498D-02-0.573D-01-0.153D+00-0.365D-01 0.452D+00 0.772D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=3.50D-07 MaxDP=1.86D-05 DE=-2.10D-08 OVMax= 2.59D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 6.10D-08 CP: 1.00D+00 1.22D+00 1.53D+00 2.55D+00 3.00D+00

CP: 3.00D+00 2.18D+00 2.53D+00 1.67D+00 1.96D+00

CP: 1.70D+00 1.16D+00

E= -1275.84174792205 Delta-E= -0.000000006621 Rises=F Damp=F

DIIS: error= 1.13D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84174792205 IErMin=13 ErrMin= 1.13D-06

ErrMax= 1.13D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.33D-09 BMatP= 5.40D-09

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

Coeff-Com: 0.105D-03-0.962D-03-0.267D-02-0.664D-02-0.114D-01 0.192D-01

Coeff-Com: 0.157D-01 0.183D-01-0.633D-01-0.144D+00-0.484D-02 0.422D+00

Coeff-Com: 0.759D+00

Coeff: 0.105D-03-0.962D-03-0.267D-02-0.664D-02-0.114D-01 0.192D-01

Coeff: 0.157D-01 0.183D-01-0.633D-01-0.144D+00-0.484D-02 0.422D+00

Coeff: 0.759D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=1.87D-07 MaxDP=9.84D-06 DE=-6.62D-09 OVMax= 1.37D-04

Cycle 14 Pass 1 IDiag 1:

RMSU= 3.75D-08 CP: 1.00D+00 1.22D+00 1.53D+00 2.56D+00 3.00D+00

CP: 3.00D+00 2.20D+00 2.57D+00 1.70D+00 2.07D+00

CP: 1.85D+00 1.39D+00 1.07D+00

E= -1275.84174792348 Delta-E= -0.000000001435 Rises=F Damp=F

DIIS: error= 5.21D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84174792348 IErMin=14 ErrMin= 5.21D-07

ErrMax= 5.21D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.05D-10 BMatP= 1.33D-09

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

Coeff-Com: -0.470D-05 0.663D-03 0.206D-03-0.132D-02-0.553D-02-0.171D-02

Coeff-Com: 0.909D-02 0.254D-01 0.130D-02-0.700D-01-0.108D+00 0.458D-01

Coeff-Com: 0.414D+00 0.690D+00

Coeff: -0.470D-05 0.663D-03 0.206D-03-0.132D-02-0.553D-02-0.171D-02

Coeff: 0.909D-02 0.254D-01 0.130D-02-0.700D-01-0.108D+00 0.458D-01

Coeff: 0.414D+00 0.690D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=5.42D-08 MaxDP=2.85D-06 DE=-1.43D-09 OVMax= 3.76D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 1.55D-08 CP: 1.00D+00 1.22D+00 1.53D+00 2.56D+00 3.00D+00

CP: 3.00D+00 2.20D+00 2.58D+00 1.71D+00 2.09D+00

CP: 1.91D+00 1.47D+00 1.29D+00 1.07D+00

E= -1275.84174792365 Delta-E= -0.000000000174 Rises=F Damp=F

DIIS: error= 1.69D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.84174792365 IErMin=15 ErrMin= 1.69D-07

ErrMax= 1.69D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.57D-11 BMatP= 3.05D-10

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

Coeff-Com: -0.240D-04 0.537D-03 0.668D-03 0.580D-03-0.540D-03-0.469D-02

Coeff-Com: 0.159D-02 0.918D-02 0.124D-01-0.859D-02-0.555D-01-0.601D-01

Coeff-Com: 0.591D-01 0.365D+00 0.681D+00

Coeff: -0.240D-04 0.537D-03 0.668D-03 0.580D-03-0.540D-03-0.469D-02

Coeff: 0.159D-02 0.918D-02 0.124D-01-0.859D-02-0.555D-01-0.601D-01

Coeff: 0.591D-01 0.365D+00 0.681D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=1.82D-08 MaxDP=8.90D-07 DE=-1.74D-10 OVMax= 1.07D-05

Cycle 16 Pass 1 IDiag 1:

RMSU= 7.04D-09 CP: 1.00D+00 1.22D+00 1.53D+00 2.56D+00 3.00D+00

CP: 3.00D+00 2.20D+00 2.58D+00 1.72D+00 2.11D+00

CP: 1.92D+00 1.51D+00 1.36D+00 1.19D+00 9.39D-01

E= -1275.84174792369 Delta-E= -0.000000000030 Rises=F Damp=F

DIIS: error= 1.13D-07 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1275.84174792369 IErMin=16 ErrMin= 1.13D-07

ErrMax= 1.13D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.01D-11 BMatP= 6.57D-11

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

Coeff-Com: -0.706D-05 0.133D-04 0.198D-03 0.564D-03 0.134D-02-0.111D-02

Coeff-Com: -0.186D-02-0.370D-02 0.428D-02 0.158D-01 0.109D-01-0.315D-01

Coeff-Com: -0.826D-01-0.428D-01 0.230D+00 0.901D+00

Coeff: -0.706D-05 0.133D-04 0.198D-03 0.564D-03 0.134D-02-0.111D-02

Coeff: -0.186D-02-0.370D-02 0.428D-02 0.158D-01 0.109D-01-0.315D-01

Coeff: -0.826D-01-0.428D-01 0.230D+00 0.901D+00

Gap= 0.056 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=9.48D-09 MaxDP=4.83D-07 DE=-3.05D-11 OVMax= 5.41D-06

Error on total polarization charges = 0.06462

SCF Done: E(UB3LYP) = -1275.84174792 A.U. after 16 cycles

NFock= 16 Conv=0.95D-08 -V/T= 1.9659

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0178 S= 1.0059

<L.S>= 0.000000000000E+00

KE= 1.320863048604D+03 PE=-8.574027464507D+03 EE= 3.216322932114D+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 2.0178, after 2.0002

Leave Link 502 at Tue Sep 17 14:29:20 2019, MaxMem= 2415919104 cpu: 1474.7

(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= 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 = 249

Leave Link 701 at Tue Sep 17 14:29:24 2019, MaxMem= 2415919104 cpu: 68.2

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 14:29:24 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 14:29:34 2019, MaxMem= 2415919104 cpu: 176.2

(Enter /home/blab/g09/l716.exe)

Dipole =-1.81188398D-13 1.38111744D-13 1.11022302D-15

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.001215821 0.005734718 -0.000000000

2 7 -0.001996918 0.005380168 -0.000000000

3 6 0.006170739 0.004840785 0.000000000

4 6 -0.007901695 -0.005369770 0.000000000

5 6 0.005314588 -0.006967899 -0.000000000

6 7 -0.006799584 -0.003584964 -0.000000000

7 6 0.004244963 0.003980811 -0.000000000

8 7 -0.001327444 0.004292207 0.000000000

9 6 -0.003685659 -0.007979735 0.000000000

10 6 0.000293225 -0.002729113 0.000000000

11 6 0.000925995 -0.000294131 -0.000000000

12 7 0.000124214 -0.008182719 0.000000000

13 6 -0.000293225 0.002729113 0.000000000

14 6 -0.000925995 0.000294131 -0.000000000

15 6 -0.004244963 -0.003980811 -0.000000000

16 7 0.001327444 -0.004292207 0.000000000

17 6 0.003685659 0.007979735 0.000000000

18 7 0.006799584 0.003584964 -0.000000000

19 7 0.001996918 -0.005380168 0.000000000

20 6 -0.006170739 -0.004840785 0.000000000

21 6 0.007901695 0.005369770 -0.000000000

22 6 -0.005314588 0.006967899 0.000000000

23 6 -0.001215821 -0.005734718 0.000000000

24 7 -0.000124214 0.008182719 -0.000000000

25 30 -0.000000000 -0.000000000 0.000000000

26 6 -0.000871529 0.000045996 -0.000000000

27 1 0.000275711 0.000084913 0.000000000

28 6 -0.001130866 -0.000889371 -0.000000000

29 1 0.000233190 -0.000881989 -0.000000000

30 6 0.001130866 0.000889371 0.000000000

31 1 -0.000233190 0.000881989 0.000000000

32 6 0.000871529 -0.000045996 0.000000000

33 1 -0.000275711 -0.000084913 -0.000000000

34 1 0.000214941 -0.000402322 -0.000000000

35 1 0.000497210 -0.000263940 -0.000156892

36 1 0.000497210 -0.000263940 0.000156892

37 1 0.000316986 0.000439161 -0.000088095

38 1 0.000316986 0.000439161 0.000088095

39 1 0.000425484 0.000174187 -0.000000000

40 1 -0.000316986 -0.000439161 -0.000088095

41 1 -0.000316986 -0.000439161 0.000088095

42 1 -0.000425484 -0.000174187 0.000000000

43 1 -0.000497210 0.000263940 -0.000156892

44 1 -0.000497210 0.000263940 0.000156892

45 1 -0.000214941 0.000402322 -0.000000000

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

Cartesian Forces: Max 0.008182719 RMS 0.002901285

Leave Link 716 at Tue Sep 17 14:29:34 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 0.007549233 RMS 0.001388520

Search for a local minimum.

Step number 23 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 12 13 14 15

16 17 18 19 20

21 22 23

DE= 9.21D-04 DEPred=-1.31D-04 R=-7.04D+00

Trust test=-7.04D+00 RLast= 1.02D-01 DXMaxT set to 5.01D-02

ITU= -1 1 0 0 1 -1 -1 1 1 -1 1 1 1 -1 0 1 -1 1 1 1

ITU= 1 0 0

Eigenvalues --- 0.00040 0.00878 0.00878 0.00878 0.00878

Eigenvalues --- 0.01335 0.01336 0.01343 0.01344 0.01606

Eigenvalues --- 0.01625 0.01634 0.01642 0.01773 0.01792

Eigenvalues --- 0.01806 0.01820 0.01888 0.01909 0.01938

Eigenvalues --- 0.01951 0.01998 0.02000 0.02044 0.02049

Eigenvalues --- 0.02070 0.02087 0.02102 0.02110 0.02114

Eigenvalues --- 0.02206 0.02312 0.02318 0.02351 0.02373

Eigenvalues --- 0.07249 0.07249 0.07260 0.07260 0.07313

Eigenvalues --- 0.07314 0.07399 0.07520 0.10292 0.14487

Eigenvalues --- 0.14507 0.14652 0.15039 0.15574 0.15960

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16034 0.16154 0.16367 0.18076 0.19714

Eigenvalues --- 0.22066 0.22109 0.22710 0.22873 0.23842

Eigenvalues --- 0.23857 0.24142 0.24805 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25185

Eigenvalues --- 0.25928 0.27401 0.28900 0.31379 0.32358

Eigenvalues --- 0.33196 0.33210 0.33282 0.33282 0.33605

Eigenvalues --- 0.33714 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33724 0.34084 0.34380 0.34437

Eigenvalues --- 0.34437 0.34442 0.35486 0.35551 0.35552

Eigenvalues --- 0.35681 0.35682 0.35682 0.35920 0.36869

Eigenvalues --- 0.37862 0.38929 0.41591 0.41820 0.43294

Eigenvalues --- 0.46405 0.48949 0.49012 0.49629 0.51356

Eigenvalues --- 0.51362 0.52064 0.53534 0.54003 0.54036

Eigenvalues --- 0.54417 0.56314 0.56343 0.57144

Cosine: 0.837 < 0.840

Cut down GDIIS temporarily because of the cosine check. E 6

DIIS coeff's: 0.05750 0.94250

Cosine: 1.000 > 0.970

Length: 0.997

GDIIS step was calculated using 2 of the last 23 vectors.

Maximum step size ( 0.050) exceeded in Quadratic search.

-- Step size scaled by 0.058

Iteration 1 RMS(Cart)= 0.00614376 RMS(Int)= 0.00002116

Iteration 2 RMS(Cart)= 0.00003342 RMS(Int)= 0.00000194

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000194

ITry= 1 IFail=0 DXMaxC= 2.60D-02 DCOld= 1.00D+10 DXMaxT= 5.01D-02 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 4.08D-10 for atom 33.

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

(Linear) (Quad) (Total)

R1 2.59411 -0.00146 -0.00067 -0.00579 -0.00647 2.58764

R2 2.70792 0.00678 0.00140 0.00331 0.00472 2.71263

R3 2.58988 -0.00095 -0.00019 -0.00210 -0.00229 2.58759

R4 2.55116 0.00168 0.00056 0.00789 0.00845 2.55961

R5 3.81094 -0.00128 -0.00058 0.00023 -0.00035 3.81059

R6 2.75559 0.00618 0.00115 -0.00798 -0.00683 2.74876

R7 2.59443 -0.00436 -0.00081 -0.00704 -0.00785 2.58658

R8 2.61415 -0.00519 -0.00095 0.00270 0.00175 2.61590

R9 2.81145 0.00094 0.00009 0.00269 0.00279 2.81424

R10 2.04342 -0.00028 -0.00001 0.00010 0.00009 2.04352

R11 2.49180 0.00377 0.00028 0.00496 0.00525 2.49705

R12 2.57297 0.00098 0.00052 0.00310 0.00362 2.57659

R13 2.80622 -0.00016 -0.00029 -0.00939 -0.00969 2.79653

R14 2.59185 -0.00262 -0.00080 -0.00283 -0.00363 2.58822

R15 3.79224 -0.00155 -0.00043 0.00271 0.00228 3.79453

R16 2.83087 0.00258 0.00064 -0.01079 -0.01015 2.82072

R17 2.47029 0.00755 0.00095 0.00870 0.00966 2.47995

R18 2.55148 -0.00101 -0.00010 0.00759 0.00750 2.55897

R19 2.80887 -0.00002 -0.00011 0.00235 0.00224 2.81111

R20 2.04132 0.00088 0.00012 0.00052 0.00064 2.04196

R21 2.47029 0.00755 0.00095 0.00870 0.00966 2.47995

R22 2.55148 -0.00101 -0.00010 0.00759 0.00750 2.55897

R23 2.83087 0.00258 0.00064 -0.01079 -0.01015 2.82072

R24 2.80887 -0.00002 -0.00011 0.00235 0.00224 2.81111

R25 2.80622 -0.00016 -0.00029 -0.00939 -0.00969 2.79653

R26 2.04132 0.00088 0.00012 0.00052 0.00064 2.04196

R27 2.57297 0.00098 0.00052 0.00310 0.00362 2.57659

R28 2.49180 0.00377 0.00028 0.00496 0.00525 2.49705

R29 2.59185 -0.00262 -0.00080 -0.00283 -0.00363 2.58822

R30 3.79224 -0.00155 -0.00043 0.00271 0.00228 3.79453

R31 2.59443 -0.00436 -0.00081 -0.00704 -0.00785 2.58658

R32 2.55116 0.00168 0.00056 0.00789 0.00845 2.55961

R33 2.59411 -0.00146 -0.00067 -0.00579 -0.00647 2.58764

R34 3.81094 -0.00128 -0.00058 0.00023 -0.00035 3.81059

R35 2.75559 0.00618 0.00115 -0.00798 -0.00683 2.74876

R36 2.61415 -0.00519 -0.00095 0.00270 0.00175 2.61590

R37 2.81145 0.00094 0.00009 0.00269 0.00279 2.81424

R38 2.70792 0.00678 0.00140 0.00331 0.00472 2.71263

R39 2.04342 -0.00028 -0.00001 0.00010 0.00009 2.04352

R40 2.58988 -0.00095 -0.00019 -0.00210 -0.00229 2.58759

R41 2.06222 0.00008 0.00002 0.00055 0.00056 2.06278

R42 2.06897 0.00021 0.00004 0.00136 0.00140 2.07037

R43 2.06897 0.00021 0.00004 0.00136 0.00140 2.07037

R44 2.06769 0.00024 0.00007 0.00165 0.00172 2.06941

R45 2.06769 0.00024 0.00007 0.00165 0.00172 2.06941

R46 2.06128 0.00013 0.00002 0.00057 0.00059 2.06187

R47 2.06769 0.00024 0.00007 0.00165 0.00172 2.06941

R48 2.06769 0.00024 0.00007 0.00165 0.00172 2.06941

R49 2.06128 0.00013 0.00002 0.00057 0.00059 2.06187

R50 2.06897 0.00021 0.00004 0.00136 0.00140 2.07037

R51 2.06897 0.00021 0.00004 0.00136 0.00140 2.07037

R52 2.06222 0.00008 0.00002 0.00055 0.00056 2.06278

A1 1.89167 0.00057 -0.00002 0.00130 0.00128 1.89295

A2 2.20409 -0.00079 -0.00002 0.00401 0.00399 2.20808

A3 2.18743 0.00023 0.00003 -0.00531 -0.00527 2.18216

A4 1.91068 -0.00202 -0.00015 -0.00164 -0.00178 1.90890

A5 2.17792 0.00212 0.00080 -0.00285 -0.00205 2.17586

A6 2.19458 -0.00010 -0.00065 0.00449 0.00383 2.19842

A7 1.89135 0.00197 0.00020 0.00114 0.00134 1.89269

A8 2.21911 0.00040 0.00030 -0.00580 -0.00551 2.21360

A9 2.17273 -0.00236 -0.00050 0.00466 0.00417 2.17690

A10 1.85783 -0.00186 -0.00038 0.00085 0.00047 1.85830

A11 2.17740 0.00046 -0.00028 0.00786 0.00758 2.18498

A12 2.24796 0.00140 0.00066 -0.00871 -0.00805 2.23991

A13 1.87324 0.00135 0.00035 -0.00165 -0.00131 1.87193

A14 2.18856 -0.00061 -0.00047 0.00395 0.00348 2.19204

A15 2.22138 -0.00074 0.00013 -0.00230 -0.00217 2.21921

A16 2.16244 0.00019 0.00037 0.00541 0.00578 2.16822

A17 2.23681 -0.00088 -0.00031 -0.00351 -0.00381 2.23300

A18 2.17045 -0.00091 -0.00011 0.00337 0.00325 2.17371

A19 1.87592 0.00179 0.00042 0.00014 0.00056 1.87648

A20 1.92070 -0.00105 -0.00029 -0.00125 -0.00154 1.91916

A21 2.19470 -0.00013 -0.00037 0.00145 0.00108 2.19578

A22 2.16778 0.00118 0.00066 -0.00019 0.00046 2.16824

A23 1.88099 0.00025 0.00012 0.00232 0.00243 1.88342

A24 2.24760 -0.00083 -0.00006 -0.00353 -0.00358 2.24401

A25 2.15460 0.00058 -0.00006 0.00121 0.00115 2.15575

A26 1.85592 0.00056 0.00008 -0.00050 -0.00043 1.85549

A27 2.16034 -0.00078 -0.00041 0.00876 0.00835 2.16869

A28 2.26693 0.00022 0.00034 -0.00825 -0.00792 2.25901

A29 1.89126 -0.00154 -0.00033 -0.00070 -0.00102 1.89023

A30 2.16557 0.00052 -0.00005 0.00450 0.00445 2.17001

A31 2.22636 0.00102 0.00038 -0.00380 -0.00342 2.22294

A32 2.18612 -0.00116 -0.00072 0.00053 -0.00019 2.18593

A33 1.85592 0.00056 0.00008 -0.00050 -0.00043 1.85549

A34 2.26693 0.00022 0.00034 -0.00825 -0.00792 2.25901

A35 2.16034 -0.00078 -0.00041 0.00876 0.00835 2.16869

A36 1.89126 -0.00154 -0.00033 -0.00070 -0.00102 1.89023

A37 2.22636 0.00102 0.00038 -0.00380 -0.00342 2.22294

A38 2.16557 0.00052 -0.00005 0.00450 0.00445 2.17001

A39 1.87592 0.00179 0.00042 0.00014 0.00056 1.87648

A40 2.17045 -0.00091 -0.00011 0.00337 0.00325 2.17371

A41 2.23681 -0.00088 -0.00031 -0.00351 -0.00381 2.23300

A42 1.92070 -0.00105 -0.00029 -0.00125 -0.00154 1.91916

A43 2.19470 -0.00013 -0.00037 0.00145 0.00108 2.19578

A44 2.16778 0.00118 0.00066 -0.00019 0.00046 2.16824

A45 2.15460 0.00058 -0.00006 0.00121 0.00115 2.15575

A46 2.24760 -0.00083 -0.00006 -0.00353 -0.00358 2.24401

A47 1.88099 0.00025 0.00012 0.00232 0.00243 1.88342

A48 2.16244 0.00019 0.00037 0.00541 0.00578 2.16822

A49 1.91068 -0.00202 -0.00015 -0.00164 -0.00178 1.90890

A50 2.19458 -0.00010 -0.00065 0.00449 0.00383 2.19842

A51 2.17792 0.00212 0.00080 -0.00285 -0.00205 2.17586

A52 2.21911 0.00040 0.00030 -0.00580 -0.00551 2.21360

A53 2.17273 -0.00236 -0.00050 0.00466 0.00417 2.17690

A54 1.89135 0.00197 0.00020 0.00114 0.00134 1.89269

A55 1.85783 -0.00186 -0.00038 0.00085 0.00047 1.85830

A56 2.17740 0.00046 -0.00028 0.00786 0.00758 2.18498

A57 2.24796 0.00140 0.00066 -0.00871 -0.00805 2.23991

A58 1.87324 0.00135 0.00035 -0.00165 -0.00131 1.87193

A59 2.22138 -0.00074 0.00013 -0.00230 -0.00217 2.21921

A60 2.18856 -0.00061 -0.00047 0.00395 0.00348 2.19204

A61 1.89167 0.00057 -0.00002 0.00130 0.00128 1.89295

A62 2.20409 -0.00079 -0.00002 0.00401 0.00399 2.20808

A63 2.18743 0.00023 0.00003 -0.00531 -0.00527 2.18216

A64 2.18612 -0.00116 -0.00072 0.00053 -0.00019 2.18593

A65 1.55873 0.00051 0.00066 -0.00203 -0.00138 1.55735

A66 1.58287 -0.00051 -0.00066 0.00203 0.00138 1.58425

A67 1.58287 -0.00051 -0.00066 0.00203 0.00138 1.58425

A68 1.55873 0.00051 0.00066 -0.00203 -0.00138 1.55735

A69 1.93759 0.00064 0.00035 -0.00493 -0.00458 1.93301

A70 1.93973 0.00023 0.00005 0.00020 0.00025 1.93998

A71 1.93973 0.00023 0.00005 0.00020 0.00025 1.93998

A72 1.88986 -0.00026 -0.00003 0.00051 0.00048 1.89034

A73 1.88986 -0.00026 -0.00003 0.00051 0.00048 1.89034

A74 1.86446 -0.00065 -0.00042 0.00384 0.00342 1.86788

A75 1.93250 0.00030 0.00009 0.00121 0.00130 1.93380

A76 1.93250 0.00030 0.00009 0.00121 0.00130 1.93380

A77 1.93897 0.00057 0.00038 -0.00490 -0.00452 1.93445

A78 1.86539 -0.00061 -0.00045 0.00298 0.00253 1.86792

A79 1.89620 -0.00031 -0.00007 -0.00012 -0.00020 1.89600

A80 1.89620 -0.00031 -0.00007 -0.00012 -0.00020 1.89600

A81 1.93250 0.00030 0.00009 0.00121 0.00130 1.93380

A82 1.93250 0.00030 0.00009 0.00121 0.00130 1.93380

A83 1.93897 0.00057 0.00038 -0.00490 -0.00452 1.93445

A84 1.86539 -0.00061 -0.00045 0.00298 0.00253 1.86792

A85 1.89620 -0.00031 -0.00007 -0.00012 -0.00020 1.89600

A86 1.89620 -0.00031 -0.00007 -0.00012 -0.00020 1.89600

A87 1.93973 0.00023 0.00005 0.00020 0.00025 1.93998

A88 1.93973 0.00023 0.00005 0.00020 0.00025 1.93998

A89 1.93759 0.00064 0.00035 -0.00493 -0.00458 1.93301

A90 1.86446 -0.00065 -0.00042 0.00384 0.00342 1.86788

A91 1.88986 -0.00026 -0.00003 0.00051 0.00048 1.89034

A92 1.88986 -0.00026 -0.00003 0.00051 0.00048 1.89034

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 1.03699 -0.00026 -0.00023 0.00254 0.00231 1.03930

D31 -1.03699 0.00026 0.00023 -0.00254 -0.00231 -1.03930

D32 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.10460 -0.00026 -0.00023 0.00254 0.00231 -2.10229

D34 2.10460 0.00026 0.00023 -0.00254 -0.00231 2.10229

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 1.03292 -0.00019 -0.00022 0.00262 0.00240 1.03532

D64 -1.03292 0.00019 0.00022 -0.00262 -0.00240 -1.03532

D65 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D66 -2.10867 -0.00019 -0.00022 0.00262 0.00240 -2.10627

D67 2.10867 0.00019 0.00022 -0.00262 -0.00240 2.10627

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 -2.10867 -0.00019 -0.00022 0.00262 0.00240 -2.10627

D80 2.10867 0.00019 0.00022 -0.00262 -0.00240 2.10627

D81 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D82 1.03292 -0.00019 -0.00022 0.00262 0.00240 1.03532

D83 -1.03292 0.00019 0.00022 -0.00262 -0.00240 -1.03532

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

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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 1.03699 -0.00026 -0.00023 0.00254 0.00231 1.03930

D126 -1.03699 0.00026 0.00023 -0.00254 -0.00231 -1.03930

D127 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D128 -2.10460 -0.00026 -0.00023 0.00254 0.00231 -2.10229

D129 2.10460 0.00026 0.00023 -0.00254 -0.00231 2.10229

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

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D136 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

Item Value Threshold Converged?

Maximum Force 0.007549 0.000450 NO

RMS Force 0.001389 0.000300 NO

Maximum Displacement 0.026033 0.001800 NO

RMS Displacement 0.006135 0.001200 NO

Predicted change in Energy=-1.512776D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:29:34 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 -2.062461 -2.197438 0.000000

2 7 0 -0.730565 -1.879484 0.000000

3 6 0 0.003144 -3.018041 0.000000

4 6 0 -0.907475 -4.152315 0.000000

5 6 0 -2.188356 -3.627369 0.000000

6 7 0 1.368516 -3.114267 0.000000

7 6 0 2.186777 -2.076720 0.000000

8 7 0 1.861607 -0.752589 0.000000

9 6 0 3.000317 0.008473 0.000000

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11 6 0 3.663524 -2.172654 0.000000

12 7 0 -3.110482 -1.316175 0.000000

13 6 0 -4.171221 0.917278 0.000000

14 6 0 -3.663524 2.172654 0.000000

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19 7 0 0.730565 1.879484 0.000000

20 6 0 -0.003144 3.018041 0.000000

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22 6 0 2.188356 3.627369 0.000000

23 6 0 2.062461 2.197438 0.000000

24 7 0 3.110482 1.316175 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.495691 -5.583482 0.000000

27 1 0 -3.119501 -4.177241 0.000000

28 6 0 5.590633 -0.472127 0.000000

29 1 0 4.213829 -3.102584 0.000000

30 6 0 -5.590633 0.472127 0.000000

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32 6 0 0.495691 5.583482 0.000000

33 1 0 3.119501 4.177241 0.000000

34 1 0 -1.369690 -6.237443 0.000000

35 1 0 0.111291 -5.820223 0.880824

36 1 0 0.111291 -5.820223 -0.880824

37 1 0 5.805347 0.142652 0.880427

38 1 0 5.805347 0.142652 -0.880427

39 1 0 6.266098 -1.329003 0.000000

40 1 0 -5.805347 -0.142652 0.880427

41 1 0 -5.805347 -0.142652 -0.880427

42 1 0 -6.266098 1.329003 0.000000

43 1 0 -0.111291 5.820223 0.880824

44 1 0 -0.111291 5.820223 -0.880824

45 1 0 1.369690 6.237443 0.000000

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Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.369322 0.000000

3 C 2.222637 1.354489 0.000000

4 C 2.270581 2.279705 1.454581 0.000000

5 C 1.435463 2.276018 2.274633 1.384277 0.000000

6 N 3.551363 2.435329 1.368758 2.501535 3.593690

7 C 4.250953 2.924002 2.377885 3.725921 4.641799

8 N 4.181614 2.826526 2.930214 4.384740 4.966544

9 C 5.522479 4.181371 4.259440 5.708152 6.335746

10 C 6.363773 4.995333 4.667555 6.021513 6.912945

11 C 5.726039 4.403859 3.756735 4.981274 6.029983

12 N 1.369296 2.445675 3.548382 3.591230 2.488361

13 C 3.761426 4.433959 5.736904 6.029329 4.958385

14 C 4.654149 5.002207 6.355137 6.899351 5.984680

15 C 4.275965 4.215697 5.545479 6.359048 5.704089

16 N 2.956856 2.864797 4.206536 4.996844 4.392129

17 C 2.381415 2.941506 4.251856 4.642350 3.708866

18 N 5.356843 5.034335 6.283840 7.281193 6.791303

19 N 4.941891 4.032957 4.951251 6.250262 6.232619

20 C 5.607317 4.951251 6.036085 7.227158 6.995472

21 C 7.009984 6.250262 7.227158 8.500642 8.373031

22 C 7.210952 6.232619 6.995472 8.373031 8.472711

23 C 6.027430 4.941891 5.607317 7.009984 7.210952

24 N 6.253385 4.996587 5.333008 6.785894 7.246814

25 Zn 3.013715 2.016479 3.018042 4.250321 4.236356

26 C 3.730961 3.711438 2.613490 1.489230 2.586792

27 H 2.244316 3.314619 3.330865 2.212167 1.081384

28 C 7.845161 6.475970 6.140171 7.467877 8.394535

29 H 6.341223 5.093427 4.211533 5.227780 6.423657

30 C 4.424315 5.399105 6.593300 6.581598 5.327416

31 H 5.720018 6.078991 7.432692 7.972799 7.028144

32 C 8.190657 7.563040 8.615614 9.836393 9.593951

33 H 8.215185 7.176832 7.841158 9.251920 9.438500

34 H 4.098972 4.404576 3.499889 2.135744 2.735452

35 H 4.315742 4.124803 2.939349 2.143748 3.297398

36 H 4.315742 4.124803 2.939349 2.143748 3.297398

37 H 8.255518 6.897994 6.665634 8.017722 8.881863

38 H 8.255518 6.897994 6.665634 8.017722 8.881863

39 H 8.373714 7.018285 6.486713 7.709166 8.761294

40 H 4.359643 5.435545 6.540763 6.390751 5.099121

41 H 4.359643 5.435545 6.540763 6.390751 5.099121

42 H 5.486925 6.398165 7.628905 7.665487 6.418225

43 H 8.298542 7.774628 8.882784 10.042971 9.713241

44 H 8.298542 7.774628 8.882784 10.042971 9.713241

45 H 9.106419 8.384246 9.355823 10.636378 10.486859

6 7 8 9 10

6 N 0.000000

7 C 1.321384 0.000000

8 N 2.412605 1.363473 0.000000

9 C 3.523391 2.238276 1.369627 0.000000

10 C 3.561168 2.298331 2.315479 1.492660 0.000000

11 C 2.480665 1.479860 2.294230 2.279728 1.354151

12 N 4.826444 5.351578 5.003928 6.252724 7.292621

13 C 6.851427 7.027671 6.259670 7.228893 8.541777

14 C 7.298833 7.230712 6.251729 7.006459 8.422050

15 C 6.291777 6.031503 4.939069 5.584227 7.027671

16 N 5.038479 4.939069 4.015953 4.918538 6.259670

17 C 5.360285 5.584227 4.918538 6.000658 7.228893

18 N 6.803380 6.291777 5.038479 5.360285 6.851427

19 N 5.034335 4.215697 2.864797 2.941506 4.433959

20 C 6.283840 5.545479 4.206536 4.251856 5.736904

21 C 7.281193 6.359048 4.996844 4.642350 6.029329

22 C 6.791303 5.704089 4.392129 3.708866 4.958385

23 C 5.356843 4.275965 2.956856 2.381415 3.761426

24 N 4.760595 3.516385 2.416500 1.312334 2.472545

25 Zn 3.401690 3.015752 2.007977 3.000329 4.270888

26 C 3.093912 4.415090 5.375350 6.594850 6.599510

27 H 4.612181 5.706906 6.044806 7.414336 7.986363

28 C 4.980680 3.763104 3.739558 2.634523 1.487578

29 H 2.845337 2.271858 3.324970 3.339354 2.185721

30 C 7.828919 8.184419 7.552205 8.603452 9.860235

31 H 8.355346 8.233647 7.195365 7.849676 9.298836

32 C 8.741434 7.844646 6.481630 6.111782 7.467892

33 H 7.498802 6.323132 5.087781 4.170471 5.201945

34 H 4.153553 5.473580 6.365917 7.622889 7.681527

35 H 3.111055 4.370047 5.433265 6.564756 6.426333

36 H 3.111055 4.370047 5.433265 6.564756 6.426333

37 H 5.573880 4.335298 4.138803 2.943017 2.137514

38 H 5.573880 4.335298 4.138803 2.943017 2.137514

39 H 5.212819 4.147282 4.442049 3.529047 2.134954

40 H 7.814727 8.269813 7.741405 8.850859 10.045253

41 H 7.814727 8.269813 7.741405 8.850859 10.045253

42 H 8.833458 9.113180 8.390031 9.360035 10.676302

43 H 9.098945 8.271559 6.918818 6.650895 8.031793

44 H 9.098945 8.271559 6.918818 6.650895 8.031793

45 H 9.351710 8.354217 7.007320 6.438867 7.683659

11 12 13 14 15

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17 C 7.006459 1.312334 1.492660 2.279728 2.238276

18 N 7.298833 4.760595 3.561168 2.480665 1.321384

19 N 5.002207 4.996587 4.995333 4.403859 2.924002

20 C 6.355137 5.333008 4.667555 3.756735 2.377885

21 C 6.899351 6.785894 6.021513 4.981274 3.725921

22 C 5.984680 7.246814 6.912945 6.029983 4.641799

23 C 4.654149 6.253385 6.363773 5.726039 4.250953

24 N 3.532390 6.754973 7.292621 6.827937 5.351578

25 Zn 4.259323 3.377487 4.270888 4.259323 3.015752

26 C 5.378924 5.004703 7.467892 8.378116 7.844646

27 H 7.073033 2.861080 5.201945 6.373156 6.323132

28 C 2.570124 8.741957 9.860235 9.624671 8.184419

29 H 1.080558 7.539018 9.298836 9.480550 8.233647

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33 H 6.373156 8.306040 7.986363 7.073033 5.706906

34 H 6.469603 5.220080 7.683659 8.717305 8.354217

35 H 5.167105 5.607328 8.031793 8.883196 8.271559

36 H 5.167105 5.607328 8.031793 8.883196 8.271559

37 H 3.274629 9.077188 10.045253 9.723969 8.269813

38 H 3.274629 9.077188 10.045253 9.723969 8.269813

39 H 2.735898 9.376589 10.676302 10.528961 9.113180

40 H 9.723969 3.068322 2.137514 3.274629 4.335298

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42 H 10.528961 4.117630 2.134954 2.735898 4.147282

43 H 8.883196 7.790967 6.426333 5.167105 4.370047

44 H 8.883196 7.790967 6.426333 5.167105 4.370047

45 H 8.717305 8.782317 7.681527 6.469603 5.473580

16 17 18 19 20

16 N 0.000000

17 C 1.369627 0.000000

18 N 2.412605 3.523391 0.000000

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21 C 4.384740 5.708152 2.501535 2.279705 1.454581

22 C 4.966544 6.335746 3.593690 2.276018 2.274633

23 C 4.181614 5.522479 3.551363 1.369322 2.222637

24 N 5.003928 6.252724 4.826444 2.445675 3.548382

25 Zn 2.007977 3.000329 3.401690 2.016479 3.018042

26 C 6.481630 6.111782 8.741434 7.563040 8.615614

27 H 5.087781 4.170471 7.498802 7.176832 7.841158

28 C 7.552205 8.603452 7.828919 5.399105 6.593300

29 H 7.195365 7.849676 8.355346 6.078991 7.432692

30 C 3.739558 2.634523 4.980680 6.475970 6.140171

31 H 3.324970 3.339354 2.845337 5.093427 4.211533

32 C 5.375350 6.594850 3.093912 3.711438 2.613490

33 H 6.044806 7.414336 4.612181 3.314619 3.330865

34 H 7.007320 6.438867 9.351710 8.384246 9.355823

35 H 6.918818 6.650895 9.098945 7.774628 8.882784

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37 H 7.741405 8.850859 7.814727 5.435545 6.540763

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39 H 8.390031 9.360035 8.833458 6.398165 7.628905

40 H 4.138803 2.943017 5.573880 6.897994 6.665634

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43 H 5.433265 6.564756 3.111055 4.124803 2.939349

44 H 5.433265 6.564756 3.111055 4.124803 2.939349

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26 C 9.836393 9.593951 8.190657 7.785227 5.605443

27 H 9.251920 9.438500 8.215185 8.306040 5.213504

28 C 6.581598 5.327416 4.424315 3.057641 5.610533

29 H 7.972799 7.028144 5.720018 4.554427 5.232818

30 C 7.467877 8.394535 7.845161 8.741957 5.610533

31 H 5.227780 6.423657 6.341223 7.539018 5.232818

32 C 1.489230 2.586792 3.730961 5.004703 5.605443

33 H 2.212167 1.081384 2.244316 2.861080 5.213504

34 H 10.636378 10.486859 9.106419 8.782317 6.386059

35 H 10.042971 9.713241 8.298542 7.790967 5.887549

36 H 10.042971 9.713241 8.298542 7.790967 5.887549

37 H 6.390751 5.099121 4.359643 3.068322 5.873462

38 H 6.390751 5.099121 4.359643 3.068322 5.873462

39 H 7.665487 6.418225 5.486925 4.117630 6.405485

40 H 8.017722 8.881863 8.255518 9.077188 5.873462

41 H 8.017722 8.881863 8.255518 9.077188 5.873462

42 H 7.709166 8.761294 8.373714 9.376589 6.405485

43 H 2.143748 3.297398 4.315742 5.607328 5.887549

44 H 2.143748 3.297398 4.315742 5.607328 5.887549

45 H 2.135744 2.735452 4.098972 5.220080 6.386059

26 27 28 29 30

26 C 0.000000

27 H 2.976894 0.000000

28 C 7.947911 9.465426 0.000000

29 H 5.323010 7.411654 2.968988 0.000000

30 C 7.913838 5.265274 11.221065 10.435805 0.000000

31 H 9.448402 7.361617 10.435805 10.465635 2.968988

32 C 11.210885 10.408714 7.913838 9.448402 7.947911

33 H 10.408714 10.427008 5.265274 7.361617 9.465426

34 H 1.091576 2.703012 9.037973 6.403360 7.926833

35 H 1.095593 3.730049 7.707215 4.999223 8.537064

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37 H 8.559605 9.954372 1.095083 3.720166 11.434686

38 H 8.559605 9.954372 1.095083 3.720166 11.434686

39 H 7.988892 9.808258 1.091096 2.712453 11.992753

40 H 7.653119 4.926137 11.434686 10.484285 1.095083

41 H 7.653119 4.926137 11.434686 10.484285 1.095083

42 H 9.004447 6.341908 11.992753 11.378393 1.091096

43 H 11.444130 10.477331 8.537064 9.954848 7.707215

44 H 11.444130 10.477331 8.537064 9.954848 7.707215

45 H 11.967202 11.341008 7.926833 9.763464 9.037973

31 32 33 34 35

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32 C 5.323010 0.000000

33 H 7.411654 2.976894 0.000000

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35 H 9.954848 11.444130 10.477331 1.772915 0.000000

36 H 9.954848 11.444130 10.477331 1.772915 1.761647

37 H 10.484285 7.653119 4.926137 9.641676 8.244886

38 H 10.484285 7.653119 4.926137 9.641676 8.430904

39 H 11.378393 9.004447 6.341908 9.077337 7.669978

40 H 3.720166 8.559605 9.954372 7.589248 8.200087

41 H 3.720166 8.559605 9.954372 7.589248 8.387099

42 H 2.712453 7.988892 9.808258 9.012543 9.620727

43 H 4.999223 1.095593 3.730049 12.155112 11.642575

44 H 4.999223 1.095593 3.730049 12.155112 11.775099

45 H 6.403360 1.091576 2.703012 12.772117 12.155112

36 37 38 39 40

36 H 0.000000

37 H 8.430904 0.000000

38 H 8.244886 1.760853 0.000000

39 H 7.669978 1.775728 1.775728 0.000000

40 H 8.387099 11.614198 11.746923 12.161512 0.000000

41 H 8.200087 11.746923 11.614198 12.161512 1.760853

42 H 9.620727 12.161512 12.161512 12.810970 1.775728

43 H 11.775099 8.200087 8.387099 9.620727 8.244886

44 H 11.642575 8.387099 8.200087 9.620727 8.430904

45 H 12.155112 7.589248 7.589248 9.012543 9.641676

41 42 43 44 45

41 H 0.000000

42 H 1.775728 0.000000

43 H 8.430904 7.669978 0.000000

44 H 8.244886 7.669978 1.761647 0.000000

45 H 9.641676 9.077337 1.772915 1.772915 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=0 Diff= 1.24D-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

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2 7 0 2.016296 0.027119 0.000000

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6 7 0 2.374336 2.435985 0.000000

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9 6 0 -1.132374 2.778436 0.000000

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18 7 0 -2.374336 -2.435985 0.000000

19 7 0 -2.016296 -0.027119 0.000000

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21 6 0 -4.189756 -0.714961 0.000000

22 6 0 -4.183150 0.669300 0.000000

23 6 0 -2.810267 1.088521 0.000000

24 7 0 -2.386041 2.390444 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 5.362264 1.633129 0.000000

27 1 0 5.041932 -1.326479 0.000000

28 6 0 -1.657656 5.360061 0.000000

29 1 0 1.297082 5.069513 0.000000

30 6 0 1.657656 -5.360061 0.000000

31 1 0 -1.297082 -5.069513 0.000000

32 6 0 -5.362264 -1.633129 0.000000

33 1 0 -5.041932 1.326479 0.000000

34 1 0 6.296129 1.067944 0.000000

35 1 0 5.354251 2.284597 0.880824

36 1 0 5.354251 2.284597 -0.880824

37 1 0 -2.308095 5.328705 0.880427

38 1 0 -2.308095 5.328705 -0.880427

39 1 0 -1.116405 6.307446 0.000000

40 1 0 2.308095 -5.328705 0.880427

41 1 0 2.308095 -5.328705 -0.880427

42 1 0 1.116405 -6.307446 0.000000

43 1 0 -5.354251 -2.284597 0.880824

44 1 0 -5.354251 -2.284597 -0.880824

45 1 0 -6.296129 -1.067944 0.000000

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

Rotational constants (GHZ): 0.1825690 0.1817853 0.0912939

Leave Link 202 at Tue Sep 17 14:29:34 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 101 beta electrons

nuclear repulsion energy 2760.4710197626 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= -0.1141821908 Hartrees.

Nuclear repulsion after empirical dispersion term = 2760.3568375719 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 = 3500

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.63D-07

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 142

GePol: Fraction of low-weight points (<1% of avg) = 4.06%

GePol: Cavity surface area = 382.029 Ang\*\*2

GePol: Cavity volume = 379.059 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0106506517 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2760.3461869202 Hartrees.

Leave Link 301 at Tue Sep 17 14:29:34 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= 15315 LenP2D= 41242.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.82D-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 14:29:35 2019, MaxMem= 2415919104 cpu: 12.7

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:29:35 2019, MaxMem= 2415919104 cpu: 1.2

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= -0.000000 -0.000000 -0.000000

Rot= 1.000000 -0.000000 0.000000 0.000151 Ang= 0.02 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 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0179 S= 1.0059

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= -1276.14723860494

Leave Link 401 at Tue Sep 17 14:29:37 2019, MaxMem= 2415919104 cpu: 39.0

(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= 36750000.

Iteration 1 A\*A^-1 deviation from unit magnitude is 4.66D-15 for 3490.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.13D-15 for 1532 1041.

Iteration 1 A^-1\*A deviation from unit magnitude is 4.66D-15 for 3490.

Iteration 1 A^-1\*A deviation from orthogonality is 6.25D-14 for 3275 3139.

E= -1275.84128499321

DIIS: error= 5.37D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.84128499321 IErMin= 1 ErrMin= 5.37D-04

ErrMax= 5.37D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.02D-04 BMatP= 9.02D-04

IDIUse=3 WtCom= 9.95D-01 WtEn= 5.37D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.306 Goal= None Shift= 0.000

Gap= 0.392 Goal= None Shift= 0.000

RMSDP=4.33D-05 MaxDP=9.27D-04 OVMax= 7.22D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.33D-05 CP: 1.00D+00

E= -1275.84161672015 Delta-E= -0.000331726942 Rises=F Damp=F

DIIS: error= 1.72D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84161672015 IErMin= 2 ErrMin= 1.72D-04

ErrMax= 1.72D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.18D-05 BMatP= 9.02D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.72D-03

Coeff-Com: 0.872D-01 0.913D+00

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

Coeff: 0.871D-01 0.913D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.079 Goal= None Shift= 0.000

RMSDP=1.54D-05 MaxDP=8.81D-04 DE=-3.32D-04 OVMax= 5.57D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.52D-05 CP: 1.00D+00 1.05D+00

E= -1275.84160995430 Delta-E= 0.000006765851 Rises=F Damp=F

DIIS: error= 3.64D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1275.84161672015 IErMin= 2 ErrMin= 1.72D-04

ErrMax= 3.64D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.41D-04 BMatP= 8.18D-05

IDIUse=3 WtCom= 3.44D-01 WtEn= 6.56D-01

Coeff-Com: -0.190D-01 0.581D+00 0.438D+00

Coeff-En: 0.000D+00 0.566D+00 0.434D+00

Coeff: -0.652D-02 0.571D+00 0.435D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.079 Goal= None Shift= 0.000

RMSDP=9.90D-06 MaxDP=6.05D-04 DE= 6.77D-06 OVMax= 2.21D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 6.33D-06 CP: 1.00D+00 1.08D+00 5.07D-01

E= -1275.84164111927 Delta-E= -0.000031164974 Rises=F Damp=F

DIIS: error= 1.16D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84164111927 IErMin= 4 ErrMin= 1.16D-04

ErrMax= 1.16D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.43D-06 BMatP= 8.18D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.16D-03

Coeff-Com: -0.132D-01 0.188D+00 0.222D+00 0.603D+00

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

Coeff: -0.132D-01 0.188D+00 0.221D+00 0.604D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=3.83D-06 MaxDP=1.82D-04 DE=-3.12D-05 OVMax= 2.05D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.93D-06 CP: 1.00D+00 1.10D+00 6.62D-01 1.04D+00

E= -1275.84164386166 Delta-E= -0.000002742389 Rises=F Damp=F

DIIS: error= 6.53D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84164386166 IErMin= 5 ErrMin= 6.53D-05

ErrMax= 6.53D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.87D-06 BMatP= 6.43D-06

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

Coeff-Com: -0.420D-02 0.212D-01 0.644D-01 0.377D+00 0.542D+00

Coeff: -0.420D-02 0.212D-01 0.644D-01 0.377D+00 0.542D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=2.20D-06 MaxDP=9.92D-05 DE=-2.74D-06 OVMax= 1.20D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.03D-06 CP: 1.00D+00 1.10D+00 7.13D-01 1.30D+00 1.13D+00

E= -1275.84164519176 Delta-E= -0.000001330100 Rises=F Damp=F

DIIS: error= 3.84D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84164519176 IErMin= 6 ErrMin= 3.84D-05

ErrMax= 3.84D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.92D-07 BMatP= 1.87D-06

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

Coeff-Com: 0.495D-02-0.763D-01-0.805D-01-0.122D+00 0.333D-01 0.124D+01

Coeff: 0.495D-02-0.763D-01-0.805D-01-0.122D+00 0.333D-01 0.124D+01

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=4.03D-06 MaxDP=1.87D-04 DE=-1.33D-06 OVMax= 2.71D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 9.36D-07 CP: 1.00D+00 1.12D+00 8.32D-01 1.70D+00 1.85D+00

CP: 1.93D+00

E= -1275.84164660283 Delta-E= -0.000001411065 Rises=F Damp=F

DIIS: error= 3.13D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84164660283 IErMin= 7 ErrMin= 3.13D-05

ErrMax= 3.13D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.52D-07 BMatP= 3.92D-07

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

Coeff-Com: 0.553D-02-0.641D-01-0.943D-01-0.258D+00-0.307D+00 0.899D+00

Coeff-Com: 0.819D+00

Coeff: 0.553D-02-0.641D-01-0.943D-01-0.258D+00-0.307D+00 0.899D+00

Coeff: 0.819D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=3.41D-06 MaxDP=1.47D-04 DE=-1.41D-06 OVMax= 2.31D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 5.54D-07 CP: 1.00D+00 1.13D+00 9.28D-01 2.04D+00 2.41D+00

CP: 3.00D+00 1.54D+00

E= -1275.84164733301 Delta-E= -0.000000730184 Rises=F Damp=F

DIIS: error= 1.67D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84164733301 IErMin= 8 ErrMin= 1.67D-05

ErrMax= 1.67D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.43D-08 BMatP= 3.52D-07

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

Coeff-Com: 0.226D-03 0.113D-01-0.885D-02-0.353D-01-0.182D+00-0.113D+00

Coeff-Com: 0.358D+00 0.969D+00

Coeff: 0.226D-03 0.113D-01-0.885D-02-0.353D-01-0.182D+00-0.113D+00

Coeff: 0.358D+00 0.969D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=2.24D-06 MaxDP=1.10D-04 DE=-7.30D-07 OVMax= 1.66D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 8.43D-07 CP: 1.00D+00 1.14D+00 9.84D-01 2.23D+00 2.80D+00

CP: 3.00D+00 2.29D+00 1.83D+00

E= -1275.84164757155 Delta-E= -0.000000238536 Rises=F Damp=F

DIIS: error= 1.01D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84164757155 IErMin= 9 ErrMin= 1.01D-05

ErrMax= 1.01D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.56D-08 BMatP= 9.43D-08

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

Coeff-Com: -0.152D-02 0.254D-01 0.192D-01 0.641D-01-0.133D-01-0.307D+00

Coeff-Com: -0.664D-01 0.558D+00 0.722D+00

Coeff: -0.152D-02 0.254D-01 0.192D-01 0.641D-01-0.133D-01-0.307D+00

Coeff: -0.664D-01 0.558D+00 0.722D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=9.69D-07 MaxDP=5.26D-05 DE=-2.39D-07 OVMax= 7.28D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 2.26D-07 CP: 1.00D+00 1.14D+00 1.00D+00 2.30D+00 2.95D+00

CP: 3.00D+00 2.67D+00 2.43D+00 1.43D+00

E= -1275.84164763601 Delta-E= -0.000000064465 Rises=F Damp=F

DIIS: error= 6.00D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84164763601 IErMin=10 ErrMin= 6.00D-06

ErrMax= 6.00D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.46D-08 BMatP= 4.56D-08

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

Coeff-Com: -0.812D-03 0.834D-02 0.104D-01 0.522D-01 0.623D-01-0.101D+00

Coeff-Com: -0.206D+00-0.817D-01 0.349D+00 0.907D+00

Coeff: -0.812D-03 0.834D-02 0.104D-01 0.522D-01 0.623D-01-0.101D+00

Coeff: -0.206D+00-0.817D-01 0.349D+00 0.907D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=7.52D-07 MaxDP=4.06D-05 DE=-6.45D-08 OVMax= 5.77D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 2.35D-07 CP: 1.00D+00 1.14D+00 1.02D+00 2.35D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.95D+00 1.80D+00 1.25D+00

E= -1275.84164766657 Delta-E= -0.000000030560 Rises=F Damp=F

DIIS: error= 3.43D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84164766657 IErMin=11 ErrMin= 3.43D-06

ErrMax= 3.43D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.83D-09 BMatP= 1.46D-08

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

Coeff-Com: 0.125D-03-0.504D-02-0.293D-02 0.871D-02 0.353D-01 0.699D-01

Coeff-Com: -0.107D+00-0.221D+00-0.105D+00 0.482D+00 0.846D+00

Coeff: 0.125D-03-0.504D-02-0.293D-02 0.871D-02 0.353D-01 0.699D-01

Coeff: -0.107D+00-0.221D+00-0.105D+00 0.482D+00 0.846D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=4.42D-07 MaxDP=2.50D-05 DE=-3.06D-08 OVMax= 3.36D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 2.46D-07 CP: 1.00D+00 1.14D+00 1.03D+00 2.38D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.02D+00 1.70D+00

CP: 1.77D+00

E= -1275.84164767709 Delta-E= -0.000000010518 Rises=F Damp=F

DIIS: error= 1.66D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84164767709 IErMin=12 ErrMin= 1.66D-06

ErrMax= 1.66D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.01D-09 BMatP= 5.83D-09

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

Coeff-Com: 0.324D-03-0.535D-02-0.570D-02-0.116D-01-0.725D-02 0.706D-01

Coeff-Com: -0.312D-03-0.699D-01-0.181D+00-0.541D-01 0.452D+00 0.813D+00

Coeff: 0.324D-03-0.535D-02-0.570D-02-0.116D-01-0.725D-02 0.706D-01

Coeff: -0.312D-03-0.699D-01-0.181D+00-0.541D-01 0.452D+00 0.813D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=3.04D-07 MaxDP=1.62D-05 DE=-1.05D-08 OVMax= 2.33D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 5.33D-08 CP: 1.00D+00 1.14D+00 1.04D+00 2.40D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.16D+00 1.94D+00

CP: 2.37D+00 1.60D+00

E= -1275.84164768061 Delta-E= -0.000000003518 Rises=F Damp=F

DIIS: error= 6.98D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84164768061 IErMin=13 ErrMin= 6.98D-07

ErrMax= 6.98D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.53D-10 BMatP= 2.01D-09

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

Coeff-Com: 0.137D-03-0.104D-02-0.222D-02-0.854D-02-0.187D-01 0.152D-01

Coeff-Com: 0.342D-01 0.496D-01-0.629D-01-0.219D+00-0.605D-01 0.448D+00

Coeff-Com: 0.826D+00

Coeff: 0.137D-03-0.104D-02-0.222D-02-0.854D-02-0.187D-01 0.152D-01

Coeff: 0.342D-01 0.496D-01-0.629D-01-0.219D+00-0.605D-01 0.448D+00

Coeff: 0.826D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=1.61D-07 MaxDP=8.42D-06 DE=-3.52D-09 OVMax= 1.21D-04

Cycle 14 Pass 1 IDiag 1:

RMSU= 2.95D-08 CP: 1.00D+00 1.14D+00 1.04D+00 2.41D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.23D+00 2.09D+00

CP: 2.67D+00 1.92D+00 1.18D+00

E= -1275.84164768136 Delta-E= -0.000000000750 Rises=F Damp=F

DIIS: error= 2.64D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84164768136 IErMin=14 ErrMin= 2.64D-07

ErrMax= 2.64D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.14D-10 BMatP= 5.53D-10

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

Coeff-Com: -0.216D-05 0.756D-03 0.161D-03-0.145D-02-0.848D-02-0.903D-02

Coeff-Com: 0.171D-01 0.449D-01 0.129D-01-0.104D+00-0.136D+00 0.556D-01

Coeff-Com: 0.448D+00 0.679D+00

Coeff: -0.216D-05 0.756D-03 0.161D-03-0.145D-02-0.848D-02-0.903D-02

Coeff: 0.171D-01 0.449D-01 0.129D-01-0.104D+00-0.136D+00 0.556D-01

Coeff: 0.448D+00 0.679D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=3.41D-08 MaxDP=1.81D-06 DE=-7.50D-10 OVMax= 2.38D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 1.22D-08 CP: 1.00D+00 1.14D+00 1.04D+00 2.41D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.25D+00 2.12D+00

CP: 2.74D+00 1.98D+00 1.28D+00 1.09D+00

E= -1275.84164768145 Delta-E= -0.000000000095 Rises=F Damp=F

DIIS: error= 1.37D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.84164768145 IErMin=15 ErrMin= 1.37D-07

ErrMax= 1.37D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.29D-11 BMatP= 1.14D-10

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

Coeff-Com: -0.251D-04 0.599D-03 0.497D-03 0.566D-03-0.147D-02-0.780D-02

Coeff-Com: 0.429D-02 0.156D-01 0.176D-01-0.233D-01-0.675D-01-0.416D-01

Coeff-Com: 0.104D+00 0.365D+00 0.634D+00

Coeff: -0.251D-04 0.599D-03 0.497D-03 0.566D-03-0.147D-02-0.780D-02

Coeff: 0.429D-02 0.156D-01 0.176D-01-0.233D-01-0.675D-01-0.416D-01

Coeff: 0.104D+00 0.365D+00 0.634D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=1.33D-08 MaxDP=6.84D-07 DE=-9.50D-11 OVMax= 8.84D-06

Cycle 16 Pass 1 IDiag 1:

RMSU= 4.57D-09 CP: 1.00D+00 1.14D+00 1.04D+00 2.42D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.25D+00 2.13D+00

CP: 2.76D+00 2.01D+00 1.32D+00 1.18D+00 1.04D+00

E= -1275.84164768144 Delta-E= 0.000000000013 Rises=F Damp=F

DIIS: error= 5.37D-08 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=15 EnMin= -1275.84164768145 IErMin=16 ErrMin= 5.37D-08

ErrMax= 5.37D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.72D-12 BMatP= 2.29D-11

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

Coeff-Com: -0.878D-05 0.995D-04 0.177D-03 0.447D-03 0.107D-02-0.142D-02

Coeff-Com: -0.882D-03-0.238D-02 0.502D-02 0.959D-02-0.425D-02-0.232D-01

Coeff-Com: -0.365D-01 0.207D-01 0.275D+00 0.756D+00

Coeff: -0.878D-05 0.995D-04 0.177D-03 0.447D-03 0.107D-02-0.142D-02

Coeff: -0.882D-03-0.238D-02 0.502D-02 0.959D-02-0.425D-02-0.232D-01

Coeff: -0.365D-01 0.207D-01 0.275D+00 0.756D+00

Gap= 0.054 Goal= None Shift= 0.000

Gap= 0.078 Goal= None Shift= 0.000

RMSDP=5.14D-09 MaxDP=2.22D-07 DE= 1.32D-11 OVMax= 3.18D-06

Error on total polarization charges = 0.06463

SCF Done: E(UB3LYP) = -1275.84164768 A.U. after 16 cycles

NFock= 16 Conv=0.51D-08 -V/T= 1.9659

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0174 S= 1.0058

<L.S>= 0.000000000000E+00

KE= 1.320830600379D+03 PE=-8.572706028544D+03 EE= 3.215687593564D+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 2.0174, after 2.0002

Leave Link 502 at Tue Sep 17 14:31:00 2019, MaxMem= 2415919104 cpu: 1456.9

(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= 15315 LenP2D= 41242.

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 14:31:04 2019, MaxMem= 2415919104 cpu: 67.9

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 14:31:04 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 14:31:14 2019, MaxMem= 2415919104 cpu: 178.4

(Enter /home/blab/g09/l716.exe)

Dipole =-5.32907052D-15-5.37347944D-14 0.00000000D+00

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000228210 0.004263906 -0.000000000

2 7 -0.001277918 0.003839526 0.000000000

3 6 0.005224977 0.008235868 -0.000000000

4 6 -0.010283778 -0.006581317 0.000000000

5 6 0.006846451 -0.006560310 -0.000000000

6 7 -0.002282057 -0.002832266 0.000000000

7 6 -0.000335630 0.002864462 -0.000000000

8 7 -0.001642425 0.003563258 -0.000000000

9 6 -0.005268165 -0.001611336 -0.000000000

10 6 0.001860250 -0.007326819 0.000000000

11 6 0.004119031 0.002261794 0.000000000

12 7 -0.000859638 -0.003104208 -0.000000000

13 6 -0.001860250 0.007326819 -0.000000000

14 6 -0.004119031 -0.002261794 -0.000000000

15 6 0.000335630 -0.002864462 0.000000000

16 7 0.001642425 -0.003563258 -0.000000000

17 6 0.005268165 0.001611336 0.000000000

18 7 0.002282057 0.002832266 -0.000000000

19 7 0.001277918 -0.003839526 -0.000000000

20 6 -0.005224977 -0.008235868 0.000000000

21 6 0.010283778 0.006581317 0.000000000

22 6 -0.006846451 0.006560310 0.000000000

23 6 -0.000228210 -0.004263906 -0.000000000

24 7 0.000859638 0.003104208 -0.000000000

25 30 0.000000000 0.000000000 0.000000000

26 6 -0.000448735 0.000741202 -0.000000000

27 1 0.000182618 0.000380317 0.000000000

28 6 -0.001567769 -0.000654517 0.000000000

29 1 -0.000062516 -0.000721208 -0.000000000

30 6 0.001567769 0.000654517 -0.000000000

31 1 0.000062516 0.000721208 0.000000000

32 6 0.000448735 -0.000741202 0.000000000

33 1 -0.000182618 -0.000380317 0.000000000

34 1 0.000540149 -0.000474635 -0.000000000

35 1 0.000333994 -0.000242700 -0.000702018

36 1 0.000333994 -0.000242700 0.000702018

37 1 0.000140008 0.000238121 -0.000658949

38 1 0.000140008 0.000238121 0.000658949

39 1 0.000468278 0.000477932 0.000000000

40 1 -0.000140008 -0.000238121 -0.000658949

41 1 -0.000140008 -0.000238121 0.000658949

42 1 -0.000468278 -0.000477932 -0.000000000

43 1 -0.000333994 0.000242700 -0.000702018

44 1 -0.000333994 0.000242700 0.000702018

45 1 -0.000540149 0.000474635 0.000000000

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

Cartesian Forces: Max 0.010283778 RMS 0.002810726

Leave Link 716 at Tue Sep 17 14:31:14 2019, MaxMem= 2415919104 cpu: 0.4

(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 0.007384374 RMS 0.001335767

Search for a local minimum.

Step number 24 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 12 13 14 15

16 17 18 19 20

21 22 23 24

DE= 1.00D-04 DEPred=-1.51D-04 R=-6.63D-01

Trust test=-6.63D-01 RLast= 5.10D-02 DXMaxT set to 5.00D-02

ITU= -1 -1 1 0 0 1 -1 -1 1 1 -1 1 1 1 -1 0 1 -1 1 1

ITU= 1 1 0 0

Eigenvalues --- 0.00822 0.00878 0.00878 0.00878 0.00878

Eigenvalues --- 0.01331 0.01332 0.01339 0.01340 0.01607

Eigenvalues --- 0.01625 0.01635 0.01642 0.01772 0.01790

Eigenvalues --- 0.01804 0.01817 0.01886 0.01907 0.01937

Eigenvalues --- 0.01949 0.01997 0.02000 0.02044 0.02048

Eigenvalues --- 0.02070 0.02086 0.02101 0.02109 0.02113

Eigenvalues --- 0.02205 0.02313 0.02318 0.02352 0.02373

Eigenvalues --- 0.07226 0.07286 0.07286 0.07292 0.07292

Eigenvalues --- 0.07308 0.07331 0.07383 0.10886 0.12775

Eigenvalues --- 0.14485 0.14507 0.14867 0.15483 0.15811

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16007 0.16235 0.16591 0.17059 0.19254

Eigenvalues --- 0.22069 0.22108 0.22720 0.23843 0.23844

Eigenvalues --- 0.23860 0.24216 0.24487 0.24951 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25367 0.27201 0.28949 0.31383 0.32788

Eigenvalues --- 0.33197 0.33210 0.33242 0.33282 0.33282

Eigenvalues --- 0.33696 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33724 0.33991 0.34226 0.34427

Eigenvalues --- 0.34437 0.34437 0.34462 0.35550 0.35552

Eigenvalues --- 0.35651 0.35682 0.35682 0.35791 0.36314

Eigenvalues --- 0.38021 0.39285 0.41601 0.41803 0.43105

Eigenvalues --- 0.46606 0.48949 0.49008 0.50234 0.51356

Eigenvalues --- 0.51364 0.51896 0.52627 0.53999 0.54031

Eigenvalues --- 0.54169 0.55557 0.56320 0.56343

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 0.30514 0.69486

Cosine: 1.000 > 0.970

Length: 1.000

GDIIS step was calculated using 2 of the last 24 vectors.

Maximum step size ( 0.050) exceeded in Quadratic search.

-- Step size scaled by 0.032

Iteration 1 RMS(Cart)= 0.00651028 RMS(Int)= 0.00000723

Iteration 2 RMS(Cart)= 0.00001405 RMS(Int)= 0.00000235

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000235

ITry= 1 IFail=0 DXMaxC= 2.60D-02 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.76D-09 for atom 27.

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

(Linear) (Quad) (Total)

R1 2.58764 -0.00058 0.00015 0.00765 0.00779 2.59543

R2 2.71263 0.00606 -0.00011 0.00862 0.00852 2.72115

R3 2.58759 0.00032 0.00005 0.00063 0.00068 2.58827

R4 2.55961 0.00005 -0.00019 0.00122 0.00102 2.56064

R5 3.81059 -0.00196 0.00001 -0.00967 -0.00967 3.80092

R6 2.74876 0.00738 0.00015 0.01186 0.01201 2.76077

R7 2.58658 -0.00189 0.00018 -0.00345 -0.00327 2.58331

R8 2.61590 -0.00578 -0.00004 -0.00671 -0.00675 2.60915

R9 2.81424 0.00042 -0.00006 0.00362 0.00356 2.81779

R10 2.04352 -0.00035 -0.00000 -0.00061 -0.00061 2.04291

R11 2.49705 0.00121 -0.00012 0.00484 0.00472 2.50178

R12 2.57659 0.00044 -0.00008 -0.00125 -0.00133 2.57526

R13 2.79653 0.00199 0.00022 0.00088 0.00110 2.79763

R14 2.58822 -0.00211 0.00008 0.00577 0.00585 2.59407

R15 3.79453 -0.00210 -0.00005 -0.00589 -0.00594 3.78859

R16 2.82072 0.00487 0.00023 0.00183 0.00205 2.82277

R17 2.47995 0.00357 -0.00022 0.00367 0.00345 2.48340

R18 2.55897 -0.00381 -0.00017 -0.00244 -0.00261 2.55636

R19 2.81111 -0.00069 -0.00005 -0.00091 -0.00096 2.81015

R20 2.04196 0.00059 -0.00001 0.00172 0.00171 2.04367

R21 2.47995 0.00357 -0.00022 0.00367 0.00345 2.48340

R22 2.55897 -0.00381 -0.00017 -0.00244 -0.00261 2.55636

R23 2.82072 0.00487 0.00023 0.00183 0.00205 2.82277

R24 2.81111 -0.00069 -0.00005 -0.00091 -0.00096 2.81015

R25 2.79653 0.00199 0.00022 0.00088 0.00110 2.79763

R26 2.04196 0.00059 -0.00001 0.00172 0.00171 2.04367

R27 2.57659 0.00044 -0.00008 -0.00125 -0.00133 2.57526

R28 2.49705 0.00121 -0.00012 0.00484 0.00472 2.50178

R29 2.58822 -0.00211 0.00008 0.00577 0.00585 2.59407

R30 3.79453 -0.00210 -0.00005 -0.00589 -0.00594 3.78859

R31 2.58658 -0.00189 0.00018 -0.00345 -0.00327 2.58331

R32 2.55961 0.00005 -0.00019 0.00122 0.00102 2.56064

R33 2.58764 -0.00058 0.00015 0.00765 0.00779 2.59543

R34 3.81059 -0.00196 0.00001 -0.00967 -0.00967 3.80092

R35 2.74876 0.00738 0.00015 0.01186 0.01201 2.76077

R36 2.61590 -0.00578 -0.00004 -0.00671 -0.00675 2.60915

R37 2.81424 0.00042 -0.00006 0.00362 0.00356 2.81779

R38 2.71263 0.00606 -0.00011 0.00862 0.00852 2.72115

R39 2.04352 -0.00035 -0.00000 -0.00061 -0.00061 2.04291

R40 2.58759 0.00032 0.00005 0.00063 0.00068 2.58827

R41 2.06278 -0.00015 -0.00001 -0.00007 -0.00008 2.06270

R42 2.07037 -0.00033 -0.00003 0.00020 0.00017 2.07054

R43 2.07037 -0.00033 -0.00003 0.00020 0.00017 2.07054

R44 2.06941 -0.00037 -0.00004 -0.00034 -0.00038 2.06903

R45 2.06941 -0.00037 -0.00004 -0.00034 -0.00038 2.06903

R46 2.06187 -0.00008 -0.00001 -0.00018 -0.00019 2.06168

R47 2.06941 -0.00037 -0.00004 -0.00034 -0.00038 2.06903

R48 2.06941 -0.00037 -0.00004 -0.00034 -0.00038 2.06903

R49 2.06187 -0.00008 -0.00001 -0.00018 -0.00019 2.06168

R50 2.07037 -0.00033 -0.00003 0.00020 0.00017 2.07054

R51 2.07037 -0.00033 -0.00003 0.00020 0.00017 2.07054

R52 2.06278 -0.00015 -0.00001 -0.00007 -0.00008 2.06270

A1 1.89295 0.00002 -0.00003 -0.00285 -0.00287 1.89008

A2 2.20808 -0.00106 -0.00009 -0.00151 -0.00160 2.20648

A3 2.18216 0.00104 0.00012 0.00435 0.00447 2.18663

A4 1.90890 -0.00117 0.00004 -0.00268 -0.00264 1.90626

A5 2.17586 0.00205 0.00005 -0.00021 -0.00017 2.17569

A6 2.19842 -0.00088 -0.00009 0.00290 0.00281 2.20123

A7 1.89269 0.00124 -0.00003 0.00393 0.00390 1.89659

A8 2.21360 0.00123 0.00012 0.00104 0.00116 2.21476

A9 2.17690 -0.00247 -0.00009 -0.00497 -0.00506 2.17183

A10 1.85830 -0.00166 -0.00001 -0.00441 -0.00443 1.85387

A11 2.18498 -0.00070 -0.00017 0.00095 0.00078 2.18576

A12 2.23991 0.00236 0.00018 0.00346 0.00365 2.24356

A13 1.87193 0.00157 0.00003 0.00601 0.00604 1.87797

A14 2.19204 -0.00102 -0.00008 -0.00407 -0.00415 2.18789

A15 2.21921 -0.00054 0.00005 -0.00194 -0.00189 2.21732

A16 2.16822 -0.00059 -0.00013 -0.00336 -0.00349 2.16473

A17 2.23300 -0.00041 0.00009 -0.00335 -0.00327 2.22974

A18 2.17371 -0.00129 -0.00007 -0.00587 -0.00595 2.16775

A19 1.87648 0.00170 -0.00001 0.00922 0.00922 1.88569

A20 1.91916 -0.00110 0.00003 -0.00871 -0.00867 1.91049

A21 2.19578 -0.00014 -0.00002 0.00510 0.00507 2.20085

A22 2.16824 0.00125 -0.00001 0.00362 0.00361 2.17185

A23 1.88342 -0.00013 -0.00005 0.00236 0.00230 1.88572

A24 2.24401 -0.00003 0.00008 -0.00723 -0.00715 2.23686

A25 2.15575 0.00016 -0.00003 0.00488 0.00485 2.16060

A26 1.85549 0.00076 0.00001 0.00229 0.00229 1.85778

A27 2.16869 -0.00173 -0.00019 0.00274 0.00256 2.17125

A28 2.25901 0.00098 0.00018 -0.00503 -0.00485 2.25416

A29 1.89023 -0.00122 0.00002 -0.00516 -0.00513 1.88510

A30 2.17001 0.00018 -0.00010 0.00255 0.00245 2.17246

A31 2.22294 0.00104 0.00008 0.00261 0.00269 2.22562

A32 2.18593 -0.00140 0.00000 0.00302 0.00303 2.18895

A33 1.85549 0.00076 0.00001 0.00229 0.00229 1.85778

A34 2.25901 0.00098 0.00018 -0.00503 -0.00485 2.25416

A35 2.16869 -0.00173 -0.00019 0.00274 0.00256 2.17125

A36 1.89023 -0.00122 0.00002 -0.00516 -0.00513 1.88510

A37 2.22294 0.00104 0.00008 0.00261 0.00269 2.22562

A38 2.17001 0.00018 -0.00010 0.00255 0.00245 2.17246

A39 1.87648 0.00170 -0.00001 0.00922 0.00922 1.88569

A40 2.17371 -0.00129 -0.00007 -0.00587 -0.00595 2.16775

A41 2.23300 -0.00041 0.00009 -0.00335 -0.00327 2.22974

A42 1.91916 -0.00110 0.00003 -0.00871 -0.00867 1.91049

A43 2.19578 -0.00014 -0.00002 0.00510 0.00507 2.20085

A44 2.16824 0.00125 -0.00001 0.00362 0.00361 2.17185

A45 2.15575 0.00016 -0.00003 0.00488 0.00485 2.16060

A46 2.24401 -0.00003 0.00008 -0.00723 -0.00715 2.23686

A47 1.88342 -0.00013 -0.00005 0.00236 0.00230 1.88572

A48 2.16822 -0.00059 -0.00013 -0.00336 -0.00349 2.16473

A49 1.90890 -0.00117 0.00004 -0.00268 -0.00264 1.90626

A50 2.19842 -0.00088 -0.00009 0.00290 0.00281 2.20123

A51 2.17586 0.00205 0.00005 -0.00021 -0.00017 2.17569

A52 2.21360 0.00123 0.00012 0.00104 0.00116 2.21476

A53 2.17690 -0.00247 -0.00009 -0.00497 -0.00506 2.17183

A54 1.89269 0.00124 -0.00003 0.00393 0.00390 1.89659

A55 1.85830 -0.00166 -0.00001 -0.00441 -0.00443 1.85387

A56 2.18498 -0.00070 -0.00017 0.00095 0.00078 2.18576

A57 2.23991 0.00236 0.00018 0.00346 0.00365 2.24356

A58 1.87193 0.00157 0.00003 0.00601 0.00604 1.87797

A59 2.21921 -0.00054 0.00005 -0.00194 -0.00189 2.21732

A60 2.19204 -0.00102 -0.00008 -0.00407 -0.00415 2.18789

A61 1.89295 0.00002 -0.00003 -0.00285 -0.00287 1.89008

A62 2.20808 -0.00106 -0.00009 -0.00151 -0.00160 2.20648

A63 2.18216 0.00104 0.00012 0.00435 0.00447 2.18663

A64 2.18593 -0.00140 0.00000 0.00302 0.00303 2.18895

A65 1.55735 0.00080 0.00003 -0.00232 -0.00229 1.55506

A66 1.58425 -0.00080 -0.00003 0.00232 0.00229 1.58653

A67 1.58425 -0.00080 -0.00003 0.00232 0.00229 1.58653

A68 1.55735 0.00080 0.00003 -0.00232 -0.00229 1.55506

A69 1.93301 0.00101 0.00010 0.00244 0.00254 1.93555

A70 1.93998 0.00030 -0.00001 0.00259 0.00258 1.94256

A71 1.93998 0.00030 -0.00001 0.00259 0.00258 1.94256

A72 1.89034 -0.00041 -0.00001 -0.00107 -0.00108 1.88926

A73 1.89034 -0.00041 -0.00001 -0.00107 -0.00108 1.88926

A74 1.86788 -0.00089 -0.00008 -0.00592 -0.00600 1.86189

A75 1.93380 0.00018 -0.00003 0.00073 0.00070 1.93450

A76 1.93380 0.00018 -0.00003 0.00073 0.00070 1.93450

A77 1.93445 0.00099 0.00010 0.00201 0.00211 1.93656

A78 1.86792 -0.00072 -0.00006 -0.00344 -0.00350 1.86443

A79 1.89600 -0.00036 0.00000 -0.00012 -0.00012 1.89588

A80 1.89600 -0.00036 0.00000 -0.00012 -0.00012 1.89588

A81 1.93380 0.00018 -0.00003 0.00073 0.00070 1.93450

A82 1.93380 0.00018 -0.00003 0.00073 0.00070 1.93450

A83 1.93445 0.00099 0.00010 0.00201 0.00211 1.93656

A84 1.86792 -0.00072 -0.00006 -0.00344 -0.00350 1.86443

A85 1.89600 -0.00036 0.00000 -0.00012 -0.00012 1.89588

A86 1.89600 -0.00036 0.00000 -0.00012 -0.00012 1.89588

A87 1.93998 0.00030 -0.00001 0.00259 0.00258 1.94256

A88 1.93998 0.00030 -0.00001 0.00259 0.00258 1.94256

A89 1.93301 0.00101 0.00010 0.00244 0.00254 1.93555

A90 1.86788 -0.00089 -0.00008 -0.00592 -0.00600 1.86189

A91 1.89034 -0.00041 -0.00001 -0.00107 -0.00108 1.88926

A92 1.89034 -0.00041 -0.00001 -0.00107 -0.00108 1.88926

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 1.03930 -0.00036 -0.00005 -0.00202 -0.00207 1.03723

D31 -1.03930 0.00036 0.00005 0.00202 0.00207 -1.03723

D32 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.10229 -0.00036 -0.00005 -0.00202 -0.00207 -2.10436

D34 2.10229 0.00036 0.00005 0.00202 0.00207 2.10436

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 1.03532 -0.00033 -0.00005 -0.00168 -0.00173 1.03359

D64 -1.03532 0.00033 0.00005 0.00168 0.00173 -1.03359

D65 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D66 -2.10627 -0.00033 -0.00005 -0.00168 -0.00173 -2.10800

D67 2.10627 0.00033 0.00005 0.00168 0.00173 2.10800

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 -2.10627 -0.00033 -0.00005 -0.00168 -0.00173 -2.10800

D80 2.10627 0.00033 0.00005 0.00168 0.00173 2.10800

D81 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D82 1.03532 -0.00033 -0.00005 -0.00168 -0.00173 1.03359

D83 -1.03532 0.00033 0.00005 0.00168 0.00173 -1.03359

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 1.03930 -0.00036 -0.00005 -0.00202 -0.00207 1.03723

D126 -1.03930 0.00036 0.00005 0.00202 0.00207 -1.03723

D127 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D128 -2.10229 -0.00036 -0.00005 -0.00202 -0.00207 -2.10436

D129 2.10229 0.00036 0.00005 0.00202 0.00207 2.10436

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 0.007384 0.000450 NO

RMS Force 0.001336 0.000300 NO

Maximum Displacement 0.025991 0.001800 NO

RMS Displacement 0.006512 0.001200 NO

Predicted change in Energy=-6.973113D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:31:14 2019, MaxMem= 2415919104 cpu: 1.3

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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1 6 0 -2.060905 -2.196938 0.000000

2 7 0 -0.725493 -1.875963 0.000000

3 6 0 0.007263 -3.015777 0.000000

4 6 0 -0.904137 -4.157567 0.000000

5 6 0 -2.180860 -3.631902 0.000000

6 7 0 1.370689 -3.114960 0.000000

7 6 0 2.189217 -2.074441 0.000000

8 7 0 1.858264 -0.752468 0.000000

9 6 0 3.002725 0.005543 0.000000

10 6 0 4.172737 -0.923083 0.000000

11 6 0 3.666074 -2.177386 0.000000

12 7 0 -3.109153 -1.315386 0.000000

13 6 0 -4.172737 0.923083 0.000000

14 6 0 -3.666074 2.177386 0.000000

15 6 0 -2.189217 2.074441 0.000000

16 7 0 -1.858264 0.752468 0.000000

17 6 0 -3.002725 -0.005543 0.000000

18 7 0 -1.370689 3.114960 0.000000

19 7 0 0.725493 1.875963 0.000000

20 6 0 -0.007263 3.015777 0.000000

21 6 0 0.904137 4.157567 0.000000

22 6 0 2.180860 3.631902 0.000000

23 6 0 2.060905 2.196938 0.000000

24 7 0 3.109153 1.315386 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.488934 -5.589706 0.000000

27 1 0 -3.111581 -4.181858 0.000000

28 6 0 5.593625 -0.484388 0.000000

29 1 0 4.214721 -3.109346 0.000000

30 6 0 -5.593625 0.484388 0.000000

31 1 0 -4.214721 3.109346 0.000000

32 6 0 0.488934 5.589706 0.000000

33 1 0 3.111581 4.181858 0.000000

34 1 0 -1.359909 -6.247620 0.000000

35 1 0 0.120561 -5.827408 0.878938

36 1 0 0.120561 -5.827408 -0.878938

37 1 0 5.811305 0.130852 0.879126

38 1 0 5.811305 0.130852 -0.879126

39 1 0 6.267028 -1.342757 0.000000

40 1 0 -5.811305 -0.130852 0.879126

41 1 0 -5.811305 -0.130852 -0.879126

42 1 0 -6.267028 1.342757 0.000000

43 1 0 -0.120561 5.827408 0.878938

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45 1 0 1.359909 6.247620 0.000000

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Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.373445 0.000000

3 C 2.224369 1.355031 0.000000

4 C 2.276440 2.288588 1.460936 0.000000

5 C 1.439969 2.280661 2.273212 1.380705 0.000000

6 N 3.552267 2.434973 1.367028 2.502371 3.588973

7 C 4.251887 2.921460 2.376349 3.729377 4.639316

8 N 4.176886 2.817453 2.923828 4.384696 4.960409

9 C 5.521890 4.176084 4.254547 5.709208 6.332500

10 C 6.362468 4.990054 4.661603 6.019679 6.906945

11 C 5.727013 4.401900 3.753638 4.980757 6.025135

12 N 1.369656 2.448690 3.550124 3.597234 2.495591

13 C 3.767540 4.440512 5.743433 6.041254 4.971464

14 C 4.659536 5.007660 6.361003 6.910856 5.996139

15 C 4.273306 4.212859 5.543902 6.363125 5.706349

16 N 2.956359 2.862136 4.204744 5.001881 4.396222

17 C 2.385212 2.946906 4.256941 4.652245 3.718325

18 N 5.356553 5.032453 6.283685 7.287477 6.795331

19 N 4.934828 4.022723 4.944186 6.249734 6.227636

20 C 5.602664 4.944186 6.031572 7.229194 6.994009

21 C 7.012218 6.249734 7.229194 8.509484 8.378128

22 C 7.208879 6.227636 6.994009 8.378128 8.472747

23 C 6.024571 4.934828 5.602664 7.012218 7.208879

24 N 6.250274 4.988910 5.327354 6.786731 7.242920

25 Zn 3.012286 2.011362 3.015786 4.254742 4.236373

26 C 3.739247 3.721270 2.621321 1.491112 2.587588

27 H 2.245847 3.318218 3.329705 2.207578 1.081061

28 C 7.843765 6.470528 6.133137 7.464124 8.387458

29 H 6.341606 5.091851 4.208498 5.225081 6.416893

30 C 4.435044 5.410172 6.604627 6.598412 5.347037

31 H 5.726741 6.085064 7.439239 7.985486 7.041378

32 C 8.193504 7.563798 8.618953 9.846318 9.600305

33 H 8.212408 7.170797 7.838542 9.255917 9.437414

34 H 4.110890 4.417451 3.509126 2.139170 2.741522

35 H 4.325696 4.135488 2.947989 2.147302 3.299897

36 H 4.325696 4.135488 2.947989 2.147302 3.299897

37 H 8.256098 6.894193 6.660409 8.016268 8.877268

38 H 8.256098 6.894193 6.660409 8.016268 8.877268

39 H 8.371624 7.012821 6.479480 7.703815 8.752542

40 H 4.371164 5.448281 6.553732 6.408401 5.119604

41 H 4.371164 5.448281 6.553732 6.408401 5.119604

42 H 5.497355 6.408492 7.639604 7.682068 6.437701

43 H 8.302264 7.776914 8.887677 10.054166 9.720900

44 H 8.302264 7.776914 8.887677 10.054166 9.720900

45 H 9.111120 8.386983 9.361633 10.648653 10.494855

6 7 8 9 10

6 N 0.000000

7 C 1.323884 0.000000

8 N 2.412280 1.362770 0.000000

9 C 3.521517 2.233412 1.372724 0.000000

10 C 3.557499 2.293464 2.320753 1.493744 0.000000

11 C 2.479484 1.480441 2.301862 2.281493 1.352769

12 N 4.827779 5.352466 4.999211 6.252992 7.292450

13 C 6.858233 7.032752 6.259429 7.233888 8.547237

14 C 7.306019 7.236192 6.253188 7.013544 8.429702

15 C 6.293077 6.031907 4.936955 5.588972 7.032752

16 N 5.038168 4.936955 4.009666 4.918040 6.259429

17 C 5.366119 5.588972 4.918040 6.005461 7.233888

18 N 6.806398 6.293077 5.038168 5.366119 6.858233

19 N 5.032453 4.212859 2.862136 2.946906 4.440512

20 C 6.283685 5.543902 4.204744 4.256941 5.743433

21 C 7.287477 6.363125 5.001881 4.652245 6.041254

22 C 6.795331 5.706349 4.396222 3.718325 4.971464

23 C 5.356553 4.273306 2.956359 2.385212 3.767540

24 N 4.759225 3.512437 2.416763 1.314160 2.478296

25 Zn 3.403199 3.015954 2.004833 3.002731 4.273619

26 C 3.095572 4.419229 5.376636 6.595339 6.596102

27 H 4.607495 5.704355 6.038218 7.410740 7.980032

28 C 4.975249 3.757428 3.744968 2.636815 1.487069

29 H 2.844038 2.274576 3.332830 3.342374 2.186666

30 C 7.839450 8.192694 7.553838 8.609677 9.867259

31 H 8.362941 8.239057 7.196858 7.856534 9.306446

32 C 8.749212 7.850485 6.488316 6.123890 7.482434

33 H 7.501617 6.323926 5.091010 4.177734 5.214065

34 H 4.155685 5.478295 6.368149 7.624606 7.678598

35 H 3.113314 4.374543 5.435730 6.565266 6.422232

36 H 3.113314 4.374543 5.435730 6.565266 6.422232

37 H 5.570209 4.330786 4.144834 2.945622 2.137416

38 H 5.570209 4.330786 4.144834 2.945622 2.137416

39 H 5.207192 4.142935 4.448105 3.531796 2.135927

40 H 7.826800 8.280022 7.744777 8.858815 10.053934

41 H 7.826800 8.280022 7.744777 8.858815 10.053934

42 H 8.843414 9.120599 8.391088 9.365707 10.682824

43 H 9.108365 8.279301 6.926981 6.664951 8.048234

44 H 9.108365 8.279301 6.926981 6.664951 8.048234

45 H 9.362586 8.363280 7.017805 6.454639 7.702660

11 12 13 14 15

11 C 0.000000

12 N 6.829843 0.000000

13 C 8.429702 2.478296 0.000000

14 C 8.527863 3.536894 1.352769 0.000000

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16 N 6.253188 2.416763 2.320753 2.301862 1.362770

17 C 7.013544 1.314160 1.493744 2.281493 2.233412

18 N 7.306019 4.759225 3.557499 2.479484 1.323884

19 N 5.007660 4.988910 4.990054 4.401900 2.921460

20 C 6.361003 5.327354 4.661603 3.753638 2.376349

21 C 6.910856 6.786731 6.019679 4.980757 3.729377

22 C 5.996139 7.242920 6.906945 6.025135 4.639316

23 C 4.659536 6.250274 6.362468 5.727013 4.251887

24 N 3.536894 6.751911 7.292450 6.829843 5.352466

25 Zn 4.263931 3.375955 4.273619 4.263931 3.015954

26 C 5.376618 5.013518 7.482434 8.391778 7.850485

27 H 7.067851 2.866473 5.214065 6.383373 6.323926

28 C 2.565481 8.742362 9.867259 9.634681 8.192694

29 H 1.081463 7.540386 9.306446 9.489809 8.239057

30 C 9.634681 3.067863 1.487069 2.565481 3.757428

31 H 9.489809 4.560760 2.186666 1.081463 2.274576

32 C 8.391778 7.786304 6.596102 5.376618 4.419229

33 H 6.383373 8.301640 7.980032 7.067851 5.704355

34 H 6.467403 5.233238 7.702660 8.734937 8.363280

35 H 5.163899 5.618001 8.048234 8.898757 8.279301

36 H 5.163899 5.618001 8.048234 8.898757 8.279301

37 H 3.271520 9.079595 10.053934 9.735599 8.280022

38 H 3.271520 9.079595 10.053934 9.735599 8.280022

39 H 2.731587 9.376221 10.682824 10.538403 9.120599

40 H 9.735599 3.078573 2.137416 3.271520 4.330786

41 H 9.735599 3.078573 2.137416 3.271520 4.330786

42 H 10.538403 4.127699 2.135927 2.731587 4.142935

43 H 8.898757 7.792543 6.422232 5.163899 4.374543

44 H 8.898757 7.792543 6.422232 5.163899 4.374543

45 H 8.734937 8.784735 7.678598 6.467403 5.478295

16 17 18 19 20

16 N 0.000000

17 C 1.372724 0.000000

18 N 2.412280 3.521517 0.000000

19 N 2.817453 4.176084 2.434973 0.000000

20 C 2.923828 4.254547 1.367028 1.355031 0.000000

21 C 4.384696 5.709208 2.502371 2.288588 1.460936

22 C 4.960409 6.332500 3.588973 2.280661 2.273212

23 C 4.176886 5.521890 3.552267 1.373445 2.224369

24 N 4.999211 6.252992 4.827779 2.448690 3.550124

25 Zn 2.004833 3.002731 3.403199 2.011362 3.015786

26 C 6.488316 6.123890 8.749212 7.563798 8.618953

27 H 5.091010 4.177734 7.501617 7.170797 7.838542

28 C 7.553838 8.609677 7.839450 5.410172 6.604627

29 H 7.196858 7.856534 8.362941 6.085064 7.439239

30 C 3.744968 2.636815 4.975249 6.470528 6.133137

31 H 3.332830 3.342374 2.844038 5.091851 4.208498

32 C 5.376636 6.595339 3.095572 3.721270 2.621321

33 H 6.038218 7.410740 4.607495 3.318218 3.329705

34 H 7.017805 6.454639 9.362586 8.386983 9.361633

35 H 6.926981 6.664951 9.108365 7.776914 8.887677

36 H 6.926981 6.664951 9.108365 7.776914 8.887677

37 H 7.744777 8.858815 7.826800 5.448281 6.553732

38 H 7.744777 8.858815 7.826800 5.448281 6.553732

39 H 8.391088 9.365707 8.843414 6.408492 7.639604

40 H 4.144834 2.945622 5.570209 6.894193 6.660409

41 H 4.144834 2.945622 5.570209 6.894193 6.660409

42 H 4.448105 3.531796 5.207192 7.012821 6.479480

43 H 5.435730 6.565266 3.113314 4.135488 2.947989

44 H 5.435730 6.565266 3.113314 4.135488 2.947989

45 H 6.368149 7.624606 4.155685 4.417451 3.509126

21 22 23 24 25

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22 C 1.380705 0.000000

23 C 2.276440 1.439969 0.000000

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25 Zn 4.254742 4.236373 3.012286 3.375955 0.000000

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27 H 9.255917 9.437414 8.212408 8.301640 5.212473

28 C 6.598412 5.347037 4.435044 3.067863 5.614559

29 H 7.985486 7.041378 5.726741 4.560760 5.237547

30 C 7.464124 8.387458 7.843765 8.742362 5.614559

31 H 5.225081 6.416893 6.341606 7.540386 5.237547

32 C 1.491112 2.587588 3.739247 5.013518 5.611049

33 H 2.207578 1.081061 2.245847 2.866473 5.212473

34 H 10.648653 10.494855 9.111120 8.784735 6.393911

35 H 10.054166 9.720900 8.302264 7.792543 5.894553

36 H 10.054166 9.720900 8.302264 7.792543 5.894553

37 H 6.408401 5.119604 4.371164 3.078573 5.878882

38 H 6.408401 5.119604 4.371164 3.078573 5.878882

39 H 7.682068 6.437701 5.497355 4.127699 6.409262

40 H 8.016268 8.877268 8.256098 9.079595 5.878882

41 H 8.016268 8.877268 8.256098 9.079595 5.878882

42 H 7.703815 8.752542 8.371624 9.376221 6.409262

43 H 2.147302 3.299897 4.325696 5.618001 5.894553

44 H 2.147302 3.299897 4.325696 5.618001 5.894553

45 H 2.139170 2.741522 4.110890 5.233238 6.393911

26 27 28 29 30

26 C 0.000000

27 H 2.976628 0.000000

28 C 7.941146 9.457901 0.000000

29 H 5.317571 7.404390 2.965093 0.000000

30 C 7.934260 5.285300 11.229117 10.445983 0.000000

31 H 9.463350 7.374183 10.445983 10.475095 2.965093

32 C 11.222099 10.413798 7.934260 9.463350 7.941146

33 H 10.413798 10.424946 5.285300 7.374183 9.457901

34 H 1.091534 2.708455 9.031416 6.397285 7.952627

35 H 1.095682 3.731905 7.699014 4.992248 8.559394

36 H 1.095682 3.731905 7.699014 4.992248 8.559394

37 H 8.555154 9.949384 1.094883 3.717637 11.444225

38 H 8.555154 9.949384 1.094883 3.717637 11.444225

39 H 7.979950 9.798919 1.090995 2.707914 12.000565

40 H 7.674607 4.946921 11.444225 10.495975 1.094883

41 H 7.674607 4.946921 11.444225 10.495975 1.094883

42 H 9.024712 6.362250 12.000565 11.388076 1.090995

43 H 11.456820 10.483518 8.559394 9.971598 7.699014

44 H 11.456820 10.483518 8.559394 9.971598 7.699014

45 H 11.980839 11.347609 7.952627 9.782778 9.031416

31 32 33 34 35

31 H 0.000000

32 C 5.317571 0.000000

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34 H 9.782778 11.980839 11.347609 0.000000

35 H 9.971598 11.456820 10.483518 1.772259 0.000000

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37 H 10.495975 7.674607 4.946921 9.637638 8.239261

38 H 10.495975 7.674607 4.946921 9.637638 8.424738

39 H 11.388076 9.024712 6.362250 9.067957 7.659222

40 H 3.717637 8.555154 9.949384 7.615947 8.224220

41 H 3.717637 8.555154 9.949384 7.615947 8.410029

42 H 2.707914 7.979950 9.798919 9.038453 9.642878

43 H 4.992248 1.095682 3.731905 12.170243 11.657310

44 H 4.992248 1.095682 3.731905 12.170243 11.789106

45 H 6.397285 1.091534 2.708455 12.787823 12.170243

36 37 38 39 40

36 H 0.000000

37 H 8.424738 0.000000

38 H 8.239261 1.758253 0.000000

39 H 7.659222 1.775407 1.775407 0.000000

40 H 8.410029 11.625557 11.757764 12.170773 0.000000

41 H 8.224220 11.757764 11.625557 12.170773 1.758253

42 H 9.642878 12.170773 12.170773 12.818524 1.775407

43 H 11.789106 8.224220 8.410029 9.642878 8.239261

44 H 11.657310 8.410029 8.224220 9.642878 8.424738

45 H 12.170243 7.615947 7.615947 9.038453 9.637638

41 42 43 44 45

41 H 0.000000

42 H 1.775407 0.000000

43 H 8.424738 7.659222 0.000000

44 H 8.239261 7.659222 1.757875 0.000000

45 H 9.637638 9.067957 1.772259 1.772259 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=0 Diff= 5.26D-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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2 7 0 1.860732 0.763709 0.000000

3 6 0 2.184093 2.079592 0.000000

4 6 0 3.639776 2.203375 0.000000

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7 6 0 0.000000 3.015954 0.000000

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9 6 0 -2.069366 2.175802 0.000000

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18 7 0 -1.318293 -3.137494 0.000000

19 7 0 -1.860732 -0.763709 0.000000

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21 6 0 -3.639776 -2.203375 0.000000

22 6 0 -4.136365 -0.915064 0.000000

23 6 0 -3.012247 -0.015136 0.000000

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25 30 0 0.000000 0.000000 0.000000

26 6 0 4.393749 3.489819 0.000000

27 1 0 5.175738 0.617746 0.000000

28 6 0 -3.495815 4.393467 0.000000

29 1 0 -0.641972 5.198055 0.000000

30 6 0 3.495815 -4.393467 0.000000

31 1 0 0.641972 -5.198055 0.000000

32 6 0 -4.393749 -3.489819 0.000000

33 1 0 -5.175738 -0.617746 0.000000

34 1 0 5.470391 3.310125 0.000000

35 1 0 4.147067 4.095736 0.878938

36 1 0 4.147067 4.095736 -0.878938

37 1 0 -4.092130 4.128301 0.879126

38 1 0 -4.092130 4.128301 -0.879126

39 1 0 -3.335925 5.472682 0.000000

40 1 0 4.092130 -4.128301 0.879126

41 1 0 4.092130 -4.128301 -0.879126

42 1 0 3.335925 -5.472682 0.000000

43 1 0 -4.147067 -4.095736 0.878938

44 1 0 -4.147067 -4.095736 -0.878938

45 1 0 -5.470391 -3.310125 0.000000

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

Rotational constants (GHZ): 0.1826733 0.1813654 0.0912132

Leave Link 202 at Tue Sep 17 14:31:14 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 101 beta electrons

nuclear repulsion energy 2759.3574631129 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= -0.1141260229 Hartrees.

Nuclear repulsion after empirical dispersion term = 2759.2433370900 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 = 3522

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.23D-09

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 196

GePol: Fraction of low-weight points (<1% of avg) = 5.57%

GePol: Cavity surface area = 382.391 Ang\*\*2

GePol: Cavity volume = 381.176 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0106124871 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2759.2327246029 Hartrees.

Leave Link 301 at Tue Sep 17 14:31:14 2019, MaxMem= 2415919104 cpu: 1.9

(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= 15315 LenP2D= 41226.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.83D-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 14:31:15 2019, MaxMem= 2415919104 cpu: 12.7

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:31:15 2019, MaxMem= 2415919104 cpu: 1.2

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.982531 0.000000 0.000000 -0.186098 Ang= -21.45 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 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0174 S= 1.0058

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= -1276.14677608430

Leave Link 401 at Tue Sep 17 14:31:17 2019, MaxMem= 2415919104 cpu: 39.1

(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= 37213452.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.44D-15 for 3514.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.59D-15 for 3514 2628.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.33D-15 for 3514.

Iteration 1 A^-1\*A deviation from orthogonality is 2.32D-10 for 2216 2195.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.66D-15 for 212.

Iteration 2 A\*A^-1 deviation from orthogonality is 2.22D-15 for 2703 1358.

Iteration 2 A^-1\*A deviation from unit magnitude is 8.88D-16 for 133.

Iteration 2 A^-1\*A deviation from orthogonality is 3.34D-16 for 1747 180.

E= -1275.84379221732

DIIS: error= 6.28D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.84379221732 IErMin= 1 ErrMin= 6.28D-04

ErrMax= 6.28D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.98D-04 BMatP= 5.98D-04

IDIUse=3 WtCom= 9.94D-01 WtEn= 6.28D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.306 Goal= None Shift= 0.000

Gap= 0.393 Goal= None Shift= 0.000

RMSDP=4.48D-05 MaxDP=1.77D-03 OVMax= 5.51D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.47D-05 CP: 1.00D+00

E= -1275.84396935229 Delta-E= -0.000177134966 Rises=F Damp=F

DIIS: error= 2.26D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84396935229 IErMin= 2 ErrMin= 2.26D-04

ErrMax= 2.26D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.87D-05 BMatP= 5.98D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.26D-03

Coeff-Com: 0.514D-01 0.949D+00

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

Coeff: 0.513D-01 0.949D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=1.10D-05 MaxDP=4.51D-04 DE=-1.77D-04 OVMax= 4.78D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.10D-05 CP: 1.00D+00 9.90D-01

E= -1275.84397018568 Delta-E= -0.000000833396 Rises=F Damp=F

DIIS: error= 3.37D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1275.84397018568 IErMin= 2 ErrMin= 2.26D-04

ErrMax= 3.37D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.29D-05 BMatP= 2.87D-05

IDIUse=3 WtCom= 3.53D-01 WtEn= 6.47D-01

Coeff-Com: -0.978D-02 0.559D+00 0.451D+00

Coeff-En: 0.000D+00 0.470D+00 0.530D+00

Coeff: -0.345D-02 0.501D+00 0.502D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=5.43D-06 MaxDP=2.70D-04 DE=-8.33D-07 OVMax= 9.60D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 4.30D-06 CP: 1.00D+00 1.03D+00 7.40D-01

E= -1275.84397839959 Delta-E= -0.000008213905 Rises=F Damp=F

DIIS: error= 6.36D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84397839959 IErMin= 4 ErrMin= 6.36D-05

ErrMax= 6.36D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.56D-06 BMatP= 2.87D-05

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

Coeff-Com: -0.767D-02 0.161D+00 0.252D+00 0.595D+00

Coeff: -0.767D-02 0.161D+00 0.252D+00 0.595D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=2.92D-06 MaxDP=1.42D-04 DE=-8.21D-06 OVMax= 1.91D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.22D-06 CP: 1.00D+00 1.03D+00 9.11D-01 1.02D+00

E= -1275.84397968195 Delta-E= -0.000001282358 Rises=F Damp=F

DIIS: error= 4.37D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84397968195 IErMin= 5 ErrMin= 4.37D-05

ErrMax= 4.37D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.07D-06 BMatP= 3.56D-06

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

Coeff-Com: -0.297D-02 0.211D-01 0.814D-01 0.401D+00 0.499D+00

Coeff: -0.297D-02 0.211D-01 0.814D-01 0.401D+00 0.499D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=1.73D-06 MaxDP=8.04D-05 DE=-1.28D-06 OVMax= 1.21D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 8.31D-07 CP: 1.00D+00 1.04D+00 9.78D-01 1.30D+00 1.20D+00

E= -1275.84398030636 Delta-E= -0.000000624418 Rises=F Damp=F

DIIS: error= 3.82D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84398030636 IErMin= 6 ErrMin= 3.82D-05

ErrMax= 3.82D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.80D-07 BMatP= 1.07D-06

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

Coeff-Com: 0.240D-02-0.550D-01-0.928D-01-0.121D+00-0.669D-01 0.133D+01

Coeff: 0.240D-02-0.550D-01-0.928D-01-0.121D+00-0.669D-01 0.133D+01

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=3.42D-06 MaxDP=1.87D-04 DE=-6.24D-07 OVMax= 2.71D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.75D-07 CP: 1.00D+00 1.05D+00 1.13D+00 1.75D+00 2.07D+00

CP: 2.09D+00

E= -1275.84398101156 Delta-E= -0.000000705197 Rises=F Damp=F

DIIS: error= 2.26D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84398101156 IErMin= 7 ErrMin= 2.26D-05

ErrMax= 2.26D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.56D-07 BMatP= 1.80D-07

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

Coeff-Com: 0.333D-02-0.473D-01-0.113D+00-0.286D+00-0.378D+00 0.100D+01

Coeff-Com: 0.821D+00

Coeff: 0.333D-02-0.473D-01-0.113D+00-0.286D+00-0.378D+00 0.100D+01

Coeff: 0.821D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=2.99D-06 MaxDP=1.55D-04 DE=-7.05D-07 OVMax= 2.32D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 4.42D-07 CP: 1.00D+00 1.06D+00 1.27D+00 2.16D+00 2.76D+00

CP: 3.00D+00 1.47D+00

E= -1275.84398142137 Delta-E= -0.000000409813 Rises=F Damp=F

DIIS: error= 1.35D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84398142137 IErMin= 8 ErrMin= 1.35D-05

ErrMax= 1.35D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.95D-08 BMatP= 1.56D-07

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

Coeff-Com: 0.313D-03 0.918D-02-0.952D-02-0.740D-01-0.219D+00-0.115D+00

Coeff-Com: 0.484D+00 0.924D+00

Coeff: 0.313D-03 0.918D-02-0.952D-02-0.740D-01-0.219D+00-0.115D+00

Coeff: 0.484D+00 0.924D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=2.14D-06 MaxDP=1.17D-04 DE=-4.10D-07 OVMax= 1.68D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 8.68D-07 CP: 1.00D+00 1.06D+00 1.36D+00 2.43D+00 3.00D+00

CP: 3.00D+00 2.18D+00 2.07D+00

E= -1275.84398158349 Delta-E= -0.000000162117 Rises=F Damp=F

DIIS: error= 8.83D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84398158349 IErMin= 9 ErrMin= 8.83D-06

ErrMax= 8.83D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.27D-08 BMatP= 4.95D-08

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

Coeff-Com: -0.767D-03 0.195D-01 0.284D-01 0.507D-01-0.543D-02-0.403D+00

Coeff-Com: -0.457D-01 0.539D+00 0.817D+00

Coeff: -0.767D-03 0.195D-01 0.284D-01 0.507D-01-0.543D-02-0.403D+00

Coeff: -0.457D-01 0.539D+00 0.817D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=1.28D-06 MaxDP=6.64D-05 DE=-1.62D-07 OVMax= 9.73D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 2.74D-07 CP: 1.00D+00 1.07D+00 1.41D+00 2.59D+00 3.00D+00

CP: 3.00D+00 2.64D+00 3.00D+00 1.80D+00

E= -1275.84398163097 Delta-E= -0.000000047476 Rises=F Damp=F

DIIS: error= 3.40D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84398163097 IErMin=10 ErrMin= 3.40D-06

ErrMax= 3.40D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.04D-09 BMatP= 2.27D-08

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

Coeff-Com: -0.597D-03 0.796D-02 0.210D-01 0.651D-01 0.954D-01-0.158D+00

Coeff-Com: -0.234D+00-0.648D-01 0.442D+00 0.826D+00

Coeff: -0.597D-03 0.796D-02 0.210D-01 0.651D-01 0.954D-01-0.158D+00

Coeff: -0.234D+00-0.648D-01 0.442D+00 0.826D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=3.49D-07 MaxDP=1.80D-05 DE=-4.75D-08 OVMax= 2.35D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.74D-07 CP: 1.00D+00 1.07D+00 1.42D+00 2.63D+00 3.00D+00

CP: 3.00D+00 2.86D+00 3.00D+00 2.01D+00 1.14D+00

E= -1275.84398163894 Delta-E= -0.000000007971 Rises=F Damp=F

DIIS: error= 1.52D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84398163894 IErMin=11 ErrMin= 1.52D-06

ErrMax= 1.52D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.59D-09 BMatP= 6.04D-09

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

Coeff-Com: -0.148D-03-0.753D-03 0.418D-02 0.193D-01 0.503D-01 0.181D-01

Coeff-Com: -0.116D+00-0.159D+00 0.239D-01 0.417D+00 0.743D+00

Coeff: -0.148D-03-0.753D-03 0.418D-02 0.193D-01 0.503D-01 0.181D-01

Coeff: -0.116D+00-0.159D+00 0.239D-01 0.417D+00 0.743D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=1.57D-07 MaxDP=7.95D-06 DE=-7.97D-09 OVMax= 9.85D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 5.27D-08 CP: 1.00D+00 1.07D+00 1.43D+00 2.64D+00 3.00D+00

CP: 3.00D+00 2.92D+00 3.00D+00 2.10D+00 1.25D+00

CP: 1.43D+00

E= -1275.84398164073 Delta-E= -0.000000001788 Rises=F Damp=F

DIIS: error= 7.75D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84398164073 IErMin=12 ErrMin= 7.75D-07

ErrMax= 7.75D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.95D-10 BMatP= 1.59D-09

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

Coeff-Com: 0.832D-04-0.269D-02-0.343D-02-0.830D-02 0.149D-02 0.528D-01

Coeff-Com: -0.481D-02-0.635D-01-0.984D-01-0.445D-02 0.402D+00 0.729D+00

Coeff: 0.832D-04-0.269D-02-0.343D-02-0.830D-02 0.149D-02 0.528D-01

Coeff: -0.481D-02-0.635D-01-0.984D-01-0.445D-02 0.402D+00 0.729D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=7.55D-08 MaxDP=4.10D-06 DE=-1.79D-09 OVMax= 4.60D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 2.56D-08 CP: 1.00D+00 1.07D+00 1.43D+00 2.65D+00 3.00D+00

CP: 3.00D+00 2.95D+00 3.00D+00 2.14D+00 1.30D+00

CP: 1.64D+00 1.09D+00

E= -1275.84398164120 Delta-E= -0.000000000475 Rises=F Damp=F

DIIS: error= 3.66D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84398164120 IErMin=13 ErrMin= 3.66D-07

ErrMax= 3.66D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.26D-10 BMatP= 4.95D-10

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

Coeff-Com: 0.879D-04-0.125D-02-0.281D-02-0.894D-02-0.111D-01 0.233D-01

Coeff-Com: 0.245D-01 0.783D-02-0.560D-01-0.116D+00 0.152D-01 0.380D+00

Coeff-Com: 0.746D+00

Coeff: 0.879D-04-0.125D-02-0.281D-02-0.894D-02-0.111D-01 0.233D-01

Coeff: 0.245D-01 0.783D-02-0.560D-01-0.116D+00 0.152D-01 0.380D+00

Coeff: 0.746D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=3.04D-08 MaxDP=2.13D-06 DE=-4.75D-10 OVMax= 1.23D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 1.59D-08 CP: 1.00D+00 1.07D+00 1.43D+00 2.65D+00 3.00D+00

CP: 3.00D+00 2.96D+00 3.00D+00 2.16D+00 1.32D+00

CP: 1.72D+00 1.27D+00 1.30D+00

E= -1275.84398164133 Delta-E= -0.000000000131 Rises=F Damp=F

DIIS: error= 2.34D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84398164133 IErMin=14 ErrMin= 2.34D-07

ErrMax= 2.34D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.59D-11 BMatP= 1.26D-10

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

Coeff-Com: 0.135D-04 0.382D-03-0.310D-03-0.219D-02-0.702D-02-0.574D-02

Coeff-Com: 0.155D-01 0.278D-01 0.322D-02-0.649D-01-0.123D+00-0.427D-01

Coeff-Com: 0.366D+00 0.833D+00

Coeff: 0.135D-04 0.382D-03-0.310D-03-0.219D-02-0.702D-02-0.574D-02

Coeff: 0.155D-01 0.278D-01 0.322D-02-0.649D-01-0.123D+00-0.427D-01

Coeff: 0.366D+00 0.833D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=1.73D-08 MaxDP=1.37D-06 DE=-1.31D-10 OVMax= 8.25D-06

Cycle 15 Pass 1 IDiag 1:

RMSU= 7.12D-09 CP: 1.00D+00 1.07D+00 1.43D+00 2.65D+00 3.00D+00

CP: 3.00D+00 2.97D+00 3.00D+00 2.16D+00 1.33D+00

CP: 1.76D+00 1.38D+00 1.72D+00 1.30D+00

E= -1275.84398164134 Delta-E= -0.000000000011 Rises=F Damp=F

DIIS: error= 1.19D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.84398164134 IErMin=15 ErrMin= 1.19D-07

ErrMax= 1.19D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.48D-11 BMatP= 3.59D-11

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

Coeff-Com: -0.176D-04 0.560D-03 0.651D-03 0.148D-02-0.604D-03-0.114D-01

Coeff-Com: 0.937D-03 0.139D-01 0.205D-01-0.224D-02-0.773D-01-0.145D+00

Coeff-Com: -0.223D-01 0.521D+00 0.700D+00

Coeff: -0.176D-04 0.560D-03 0.651D-03 0.148D-02-0.604D-03-0.114D-01

Coeff: 0.937D-03 0.139D-01 0.205D-01-0.224D-02-0.773D-01-0.145D+00

Coeff: -0.223D-01 0.521D+00 0.700D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=1.31D-08 MaxDP=8.40D-07 DE=-1.09D-11 OVMax= 7.19D-06

Cycle 16 Pass 1 IDiag 1:

RMSU= 3.91D-09 CP: 1.00D+00 1.07D+00 1.43D+00 2.65D+00 3.00D+00

CP: 3.00D+00 2.97D+00 3.00D+00 2.17D+00 1.34D+00

CP: 1.78D+00 1.42D+00 1.90D+00 1.58D+00 1.08D+00

E= -1275.84398164138 Delta-E= -0.000000000040 Rises=F Damp=F

DIIS: error= 5.70D-08 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1275.84398164138 IErMin=16 ErrMin= 5.70D-08

ErrMax= 5.70D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.96D-12 BMatP= 1.48D-11

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

Coeff-Com: -0.741D-05 0.908D-04 0.274D-03 0.941D-03 0.121D-02-0.196D-02

Coeff-Com: -0.248D-02-0.158D-02 0.624D-02 0.117D-01-0.107D-02-0.394D-01

Coeff-Com: -0.839D-01 0.926D-02 0.274D+00 0.826D+00

Coeff: -0.741D-05 0.908D-04 0.274D-03 0.941D-03 0.121D-02-0.196D-02

Coeff: -0.248D-02-0.158D-02 0.624D-02 0.117D-01-0.107D-02-0.394D-01

Coeff: -0.839D-01 0.926D-02 0.274D+00 0.826D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=5.61D-09 MaxDP=2.81D-07 DE=-4.00D-11 OVMax= 3.82D-06

Error on total polarization charges = 0.06473

SCF Done: E(UB3LYP) = -1275.84398164 A.U. after 16 cycles

NFock= 16 Conv=0.56D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0181 S= 1.0060

<L.S>= 0.000000000000E+00

KE= 1.320763267727D+03 PE=-8.570406234297D+03 EE= 3.214566260327D+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 2.0181, after 2.0002

Leave Link 502 at Tue Sep 17 14:32:41 2019, MaxMem= 2415919104 cpu: 1469.1

(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= 15315 LenP2D= 41226.

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 = 246

Leave Link 701 at Tue Sep 17 14:32:45 2019, MaxMem= 2415919104 cpu: 70.5

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 14:32:45 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 14:32:55 2019, MaxMem= 2415919104 cpu: 176.8

(Enter /home/blab/g09/l716.exe)

Dipole = 3.41060513D-13 3.28626015D-14 6.66133815D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.002634914 0.003385877 0.000000000

2 7 -0.003706700 0.000976606 0.000000000

3 6 0.003300006 0.006065782 0.000000000

4 6 -0.006320291 -0.003665491 0.000000000

5 6 0.003621079 -0.003570028 -0.000000000

6 7 -0.000728360 -0.001502993 -0.000000000

7 6 -0.002743629 -0.000195780 -0.000000000

8 7 0.003324874 0.003277881 -0.000000000

9 6 -0.007159032 0.000948390 0.000000000

10 6 0.002505117 -0.005562203 0.000000000

11 6 0.001985185 0.002545005 -0.000000000

12 7 -0.001288990 -0.002195300 -0.000000000

13 6 -0.002505117 0.005562203 -0.000000000

14 6 -0.001985185 -0.002545005 0.000000000

15 6 0.002743629 0.000195780 -0.000000000

16 7 -0.003324874 -0.003277881 -0.000000000

17 6 0.007159032 -0.000948390 -0.000000000

18 7 0.000728360 0.001502993 -0.000000000

19 7 0.003706700 -0.000976606 -0.000000000

20 6 -0.003300006 -0.006065782 -0.000000000

21 6 0.006320291 0.003665491 -0.000000000

22 6 -0.003621079 0.003570028 -0.000000000

23 6 -0.002634914 -0.003385877 -0.000000000

24 7 0.001288990 0.002195300 -0.000000000

25 30 -0.000000000 0.000000000 0.000000000

26 6 -0.000111815 0.001292162 -0.000000000

27 1 -0.000161561 0.000289815 0.000000000

28 6 -0.001244148 0.000285304 -0.000000000

29 1 -0.000558704 -0.000071918 -0.000000000

30 6 0.001244148 -0.000285304 -0.000000000

31 1 0.000558704 0.000071918 0.000000000

32 6 0.000111815 -0.001292162 -0.000000000

33 1 0.000161561 -0.000289815 -0.000000000

34 1 0.000333429 -0.000224626 -0.000000000

35 1 0.000035159 0.000168415 -0.000422256

36 1 0.000035159 0.000168415 0.000422256

37 1 0.000126367 0.000183610 -0.000348735

38 1 0.000126367 0.000183610 0.000348735

39 1 0.000327618 0.000358311 -0.000000000

40 1 -0.000126367 -0.000183610 -0.000348735

41 1 -0.000126367 -0.000183610 0.000348735

42 1 -0.000327618 -0.000358311 -0.000000000

43 1 -0.000035159 -0.000168415 -0.000422256

44 1 -0.000035159 -0.000168415 0.000422256

45 1 -0.000333429 0.000224626 0.000000000

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

Cartesian Forces: Max 0.007159032 RMS 0.002119875

Leave Link 716 at Tue Sep 17 14:32:55 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 0.004061907 RMS 0.000934142

Search for a local minimum.

Step number 25 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 12 13 14 15

16 17 18 19 20

21 22 23 24 25

DE= -2.33D-03 DEPred=-6.97D-04 R= 3.35D+00

TightC=F SS= 1.41D+00 RLast= 5.06D-02 DXNew= 8.4090D-02 1.5172D-01

Trust test= 3.35D+00 RLast= 5.06D-02 DXMaxT set to 8.41D-02

ITU= 1 -1 -1 1 0 0 1 -1 -1 1 1 -1 1 1 1 -1 0 1 -1 1

ITU= 1 1 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01330

Eigenvalues --- 0.01332 0.01338 0.01338 0.01605 0.01624

Eigenvalues --- 0.01633 0.01641 0.01772 0.01789 0.01805

Eigenvalues --- 0.01817 0.01886 0.01905 0.01937 0.01948

Eigenvalues --- 0.01997 0.01998 0.02043 0.02048 0.02070

Eigenvalues --- 0.02086 0.02101 0.02109 0.02113 0.02205

Eigenvalues --- 0.02313 0.02318 0.02352 0.02373 0.04933

Eigenvalues --- 0.06986 0.07250 0.07250 0.07269 0.07269

Eigenvalues --- 0.07287 0.07379 0.07561 0.07766 0.12517

Eigenvalues --- 0.14484 0.14497 0.14511 0.15085 0.15451

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16007 0.16156 0.16328 0.17151 0.18581

Eigenvalues --- 0.20300 0.22060 0.22101 0.22961 0.23703

Eigenvalues --- 0.23845 0.23855 0.24255 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25091

Eigenvalues --- 0.25350 0.26235 0.28983 0.31544 0.32128

Eigenvalues --- 0.33197 0.33200 0.33282 0.33282 0.33556

Eigenvalues --- 0.33697 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33724 0.34175 0.34381 0.34437

Eigenvalues --- 0.34437 0.34439 0.35365 0.35551 0.35559

Eigenvalues --- 0.35673 0.35682 0.35682 0.35740 0.36870

Eigenvalues --- 0.38322 0.38589 0.41628 0.41817 0.44141

Eigenvalues --- 0.46519 0.48838 0.48945 0.49003 0.51233

Eigenvalues --- 0.51356 0.51366 0.53216 0.53996 0.54035

Eigenvalues --- 0.54326 0.56316 0.56346 0.57345

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 1.15837 -0.54102 0.38265

Cosine: 0.966 > 0.840

Length: 0.981

GDIIS step was calculated using 3 of the last 25 vectors.

Maximum step size ( 0.084) exceeded in Quadratic search.

-- Step size scaled by 0.764

Iteration 1 RMS(Cart)= 0.01010435 RMS(Int)= 0.00005114

Iteration 2 RMS(Cart)= 0.00010889 RMS(Int)= 0.00000665

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000665

ITry= 1 IFail=0 DXMaxC= 3.82D-02 DCOld= 1.00D+10 DXMaxT= 8.41D-02 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 6.75D-10 for atom 39.

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

(Linear) (Quad) (Total)

R1 2.59543 -0.00238 0.00283 -0.01797 -0.01513 2.58031

R2 2.72115 0.00237 -0.00035 0.01299 0.01264 2.73379

R3 2.58827 -0.00154 0.00075 -0.00049 0.00026 2.58853

R4 2.56064 -0.00140 -0.00235 0.00895 0.00661 2.56725

R5 3.80092 -0.00149 -0.00107 -0.00209 -0.00312 3.79780

R6 2.76077 0.00381 0.00345 0.00576 0.00921 2.76998

R7 2.58331 -0.00105 0.00190 -0.00718 -0.00530 2.57801

R8 2.60915 -0.00406 -0.00133 -0.00799 -0.00932 2.59983

R9 2.81779 -0.00130 -0.00038 -0.00162 -0.00200 2.81579

R10 2.04291 -0.00000 -0.00010 0.00036 0.00026 2.04317

R11 2.50178 0.00000 -0.00096 -0.00334 -0.00433 2.49745

R12 2.57526 0.00002 -0.00122 0.01129 0.01007 2.58533

R13 2.79763 0.00104 0.00296 -0.00316 -0.00019 2.79744

R14 2.59407 -0.00315 0.00177 -0.01837 -0.01661 2.57746

R15 3.78859 -0.00175 -0.00139 -0.00346 -0.00484 3.78375

R16 2.82277 0.00319 0.00321 0.01218 0.01539 2.83816

R17 2.48340 0.00061 -0.00241 0.00894 0.00652 2.48992

R18 2.55636 -0.00223 -0.00251 -0.00101 -0.00351 2.55285

R19 2.81015 -0.00037 -0.00077 -0.00146 -0.00224 2.80792

R20 2.04367 -0.00021 0.00002 -0.00001 0.00000 2.04367

R21 2.48340 0.00061 -0.00241 0.00894 0.00652 2.48992

R22 2.55636 -0.00223 -0.00251 -0.00101 -0.00351 2.55285

R23 2.82277 0.00319 0.00321 0.01218 0.01539 2.83816

R24 2.81015 -0.00037 -0.00077 -0.00146 -0.00224 2.80792

R25 2.79763 0.00104 0.00296 -0.00316 -0.00019 2.79744

R26 2.04367 -0.00021 0.00002 -0.00001 0.00000 2.04367

R27 2.57526 0.00002 -0.00122 0.01129 0.01007 2.58533

R28 2.50178 0.00000 -0.00096 -0.00334 -0.00433 2.49745

R29 2.59407 -0.00315 0.00177 -0.01837 -0.01661 2.57746

R30 3.78859 -0.00175 -0.00139 -0.00346 -0.00484 3.78375

R31 2.58331 -0.00105 0.00190 -0.00718 -0.00530 2.57801

R32 2.56064 -0.00140 -0.00235 0.00895 0.00661 2.56725

R33 2.59543 -0.00238 0.00283 -0.01797 -0.01513 2.58031

R34 3.80092 -0.00149 -0.00107 -0.00209 -0.00312 3.79780

R35 2.76077 0.00381 0.00345 0.00576 0.00921 2.76998

R36 2.60915 -0.00406 -0.00133 -0.00799 -0.00932 2.59983

R37 2.81779 -0.00130 -0.00038 -0.00162 -0.00200 2.81579

R38 2.72115 0.00237 -0.00035 0.01299 0.01264 2.73379

R39 2.04291 -0.00000 -0.00010 0.00036 0.00026 2.04317

R40 2.58827 -0.00154 0.00075 -0.00049 0.00026 2.58853

R41 2.06270 -0.00012 -0.00017 0.00016 -0.00001 2.06269

R42 2.07054 -0.00037 -0.00039 0.00017 -0.00022 2.07032

R43 2.07054 -0.00037 -0.00039 0.00017 -0.00022 2.07032

R44 2.06903 -0.00016 -0.00055 0.00096 0.00042 2.06944

R45 2.06903 -0.00016 -0.00055 0.00096 0.00042 2.06944

R46 2.06168 -0.00006 -0.00020 0.00043 0.00024 2.06192

R47 2.06903 -0.00016 -0.00055 0.00096 0.00042 2.06944

R48 2.06903 -0.00016 -0.00055 0.00096 0.00042 2.06944

R49 2.06168 -0.00006 -0.00020 0.00043 0.00024 2.06192

R50 2.07054 -0.00037 -0.00039 0.00017 -0.00022 2.07032

R51 2.07054 -0.00037 -0.00039 0.00017 -0.00022 2.07032

R52 2.06270 -0.00012 -0.00017 0.00016 -0.00001 2.06269

A1 1.89008 0.00078 -0.00072 0.00298 0.00227 1.89235

A2 2.20648 -0.00020 -0.00136 0.00088 -0.00047 2.20601

A3 2.18663 -0.00057 0.00208 -0.00386 -0.00180 2.18483

A4 1.90626 -0.00037 0.00020 -0.00006 0.00011 1.90637

A5 2.17569 0.00189 0.00058 0.01397 0.01457 2.19026

A6 2.20123 -0.00153 -0.00078 -0.01391 -0.01468 2.18655

A7 1.89659 0.00011 0.00008 -0.00102 -0.00093 1.89565

A8 2.21476 0.00135 0.00175 0.00338 0.00514 2.21990

A9 2.17183 -0.00146 -0.00183 -0.00236 -0.00420 2.16763

A10 1.85387 -0.00049 -0.00067 -0.00108 -0.00176 1.85212

A11 2.18576 -0.00116 -0.00212 -0.00619 -0.00831 2.17744

A12 2.24356 0.00165 0.00279 0.00728 0.01007 2.25362

A13 1.87797 -0.00003 0.00111 -0.00081 0.00031 1.87828

A14 2.18789 -0.00034 -0.00152 -0.00398 -0.00550 2.18239

A15 2.21732 0.00037 0.00041 0.00479 0.00519 2.22251

A16 2.16473 -0.00047 -0.00211 0.00954 0.00741 2.17214

A17 2.22974 0.00059 0.00072 -0.00197 -0.00127 2.22847

A18 2.16775 -0.00020 -0.00167 0.00364 0.00197 2.16973

A19 1.88569 -0.00039 0.00095 -0.00167 -0.00070 1.88499

A20 1.91049 0.00096 -0.00060 0.00214 0.00153 1.91202

A21 2.20085 -0.00152 0.00030 -0.01072 -0.01041 2.19044

A22 2.17185 0.00056 0.00030 0.00857 0.00887 2.18072

A23 1.88572 -0.00051 -0.00043 0.00109 0.00066 1.88638

A24 2.23686 0.00144 0.00018 0.00644 0.00662 2.24348

A25 2.16060 -0.00093 0.00025 -0.00753 -0.00728 2.15333

A26 1.85778 -0.00002 0.00040 -0.00209 -0.00169 1.85609

A27 2.17125 -0.00190 -0.00213 -0.00954 -0.01167 2.15958

A28 2.25416 0.00192 0.00173 0.01163 0.01336 2.26751

A29 1.88510 -0.00003 -0.00032 0.00052 0.00020 1.88530

A30 2.17246 -0.00053 -0.00100 -0.00416 -0.00516 2.16730

A31 2.22562 0.00056 0.00133 0.00364 0.00496 2.23059

A32 2.18895 -0.00212 0.00042 -0.01619 -0.01578 2.17318

A33 1.85778 -0.00002 0.00040 -0.00209 -0.00169 1.85609

A34 2.25416 0.00192 0.00173 0.01163 0.01336 2.26751

A35 2.17125 -0.00190 -0.00213 -0.00954 -0.01167 2.15958

A36 1.88510 -0.00003 -0.00032 0.00052 0.00020 1.88530

A37 2.22562 0.00056 0.00133 0.00364 0.00496 2.23059

A38 2.17246 -0.00053 -0.00100 -0.00416 -0.00516 2.16730

A39 1.88569 -0.00039 0.00095 -0.00167 -0.00070 1.88499

A40 2.16775 -0.00020 -0.00167 0.00364 0.00197 2.16973

A41 2.22974 0.00059 0.00072 -0.00197 -0.00127 2.22847

A42 1.91049 0.00096 -0.00060 0.00214 0.00153 1.91202

A43 2.20085 -0.00152 0.00030 -0.01072 -0.01041 2.19044

A44 2.17185 0.00056 0.00030 0.00857 0.00887 2.18072

A45 2.16060 -0.00093 0.00025 -0.00753 -0.00728 2.15333

A46 2.23686 0.00144 0.00018 0.00644 0.00662 2.24348

A47 1.88572 -0.00051 -0.00043 0.00109 0.00066 1.88638

A48 2.16473 -0.00047 -0.00211 0.00954 0.00741 2.17214

A49 1.90626 -0.00037 0.00020 -0.00006 0.00011 1.90637

A50 2.20123 -0.00153 -0.00078 -0.01391 -0.01468 2.18655

A51 2.17569 0.00189 0.00058 0.01397 0.01457 2.19026

A52 2.21476 0.00135 0.00175 0.00338 0.00514 2.21990

A53 2.17183 -0.00146 -0.00183 -0.00236 -0.00420 2.16763

A54 1.89659 0.00011 0.00008 -0.00102 -0.00093 1.89565

A55 1.85387 -0.00049 -0.00067 -0.00108 -0.00176 1.85212

A56 2.18576 -0.00116 -0.00212 -0.00619 -0.00831 2.17744

A57 2.24356 0.00165 0.00279 0.00728 0.01007 2.25362

A58 1.87797 -0.00003 0.00111 -0.00081 0.00031 1.87828

A59 2.21732 0.00037 0.00041 0.00479 0.00519 2.22251

A60 2.18789 -0.00034 -0.00152 -0.00398 -0.00550 2.18239

A61 1.89008 0.00078 -0.00072 0.00298 0.00227 1.89235

A62 2.20648 -0.00020 -0.00136 0.00088 -0.00047 2.20601

A63 2.18663 -0.00057 0.00208 -0.00386 -0.00180 2.18483

A64 2.18895 -0.00212 0.00042 -0.01619 -0.01578 2.17318

A65 1.55506 0.00158 0.00013 0.01367 0.01381 1.56887

A66 1.58653 -0.00158 -0.00013 -0.01367 -0.01381 1.57272

A67 1.58653 -0.00158 -0.00013 -0.01367 -0.01381 1.57272

A68 1.55506 0.00158 0.00013 0.01367 0.01381 1.56887

A69 1.93555 0.00066 0.00165 0.00363 0.00527 1.94082

A70 1.94256 -0.00018 0.00024 -0.00142 -0.00118 1.94138

A71 1.94256 -0.00018 0.00024 -0.00142 -0.00118 1.94138

A72 1.88926 -0.00008 -0.00027 0.00013 -0.00015 1.88911

A73 1.88926 -0.00008 -0.00027 0.00013 -0.00015 1.88911

A74 1.86189 -0.00016 -0.00172 -0.00117 -0.00290 1.85898

A75 1.93450 0.00013 -0.00029 -0.00027 -0.00057 1.93393

A76 1.93450 0.00013 -0.00029 -0.00027 -0.00057 1.93393

A77 1.93656 0.00066 0.00158 0.00539 0.00696 1.94352

A78 1.86443 -0.00045 -0.00116 -0.00380 -0.00496 1.85947

A79 1.89588 -0.00027 0.00004 -0.00072 -0.00068 1.89520

A80 1.89588 -0.00027 0.00004 -0.00072 -0.00068 1.89520

A81 1.93450 0.00013 -0.00029 -0.00027 -0.00057 1.93393

A82 1.93450 0.00013 -0.00029 -0.00027 -0.00057 1.93393

A83 1.93656 0.00066 0.00158 0.00539 0.00696 1.94352

A84 1.86443 -0.00045 -0.00116 -0.00380 -0.00496 1.85947

A85 1.89588 -0.00027 0.00004 -0.00072 -0.00068 1.89520

A86 1.89588 -0.00027 0.00004 -0.00072 -0.00068 1.89520

A87 1.94256 -0.00018 0.00024 -0.00142 -0.00118 1.94138

A88 1.94256 -0.00018 0.00024 -0.00142 -0.00118 1.94138

A89 1.93555 0.00066 0.00165 0.00363 0.00527 1.94082

A90 1.86189 -0.00016 -0.00172 -0.00117 -0.00290 1.85898

A91 1.88926 -0.00008 -0.00027 0.00013 -0.00015 1.88911

A92 1.88926 -0.00008 -0.00027 0.00013 -0.00015 1.88911

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 1.03723 -0.00022 -0.00093 -0.00167 -0.00260 1.03463

D31 -1.03723 0.00022 0.00093 0.00167 0.00260 -1.03463

D32 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.10436 -0.00022 -0.00093 -0.00167 -0.00260 -2.10696

D34 2.10436 0.00022 0.00093 0.00167 0.00260 2.10696

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 1.03359 -0.00020 -0.00091 -0.00254 -0.00345 1.03014

D64 -1.03359 0.00020 0.00091 0.00254 0.00345 -1.03014

D65 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D66 -2.10800 -0.00020 -0.00091 -0.00254 -0.00345 -2.11145

D67 2.10800 0.00020 0.00091 0.00254 0.00345 2.11145

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 -2.10800 -0.00020 -0.00091 -0.00254 -0.00345 -2.11145

D80 2.10800 0.00020 0.00091 0.00254 0.00345 2.11145

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 1.03359 -0.00020 -0.00091 -0.00254 -0.00345 1.03014

D83 -1.03359 0.00020 0.00091 0.00254 0.00345 -1.03014

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 1.03723 -0.00022 -0.00093 -0.00167 -0.00260 1.03463

D126 -1.03723 0.00022 0.00093 0.00167 0.00260 -1.03463

D127 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D128 -2.10436 -0.00022 -0.00093 -0.00167 -0.00260 -2.10696

D129 2.10436 0.00022 0.00093 0.00167 0.00260 2.10696

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 0.004062 0.000450 NO

RMS Force 0.000934 0.000300 NO

Maximum Displacement 0.038150 0.001800 NO

RMS Displacement 0.010133 0.001200 NO

Predicted change in Energy=-6.636533D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:32:55 2019, MaxMem= 2415919104 cpu: 1.4

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.069289 -2.192689 0.000000

2 7 0 -0.743202 -1.867239 0.000000

3 6 0 -0.002970 -3.006389 0.000000

4 6 0 -0.912866 -4.155598 0.000000

5 6 0 -2.186178 -3.634616 0.000000

6 7 0 1.357636 -3.105699 0.000000

7 6 0 2.182673 -2.073262 0.000000

8 7 0 1.858904 -0.744029 0.000000

9 6 0 2.999676 0.003607 0.000000

10 6 0 4.172143 -0.935001 0.000000

11 6 0 3.658821 -2.184583 0.000000

12 7 0 -3.121432 -1.315579 0.000000

13 6 0 -4.172143 0.935001 0.000000

14 6 0 -3.658821 2.184583 0.000000

15 6 0 -2.182673 2.073262 0.000000

16 7 0 -1.858904 0.744029 0.000000

17 6 0 -2.999676 -0.003607 0.000000

18 7 0 -1.357636 3.105699 0.000000

19 7 0 0.743202 1.867239 0.000000

20 6 0 0.002970 3.006389 0.000000

21 6 0 0.912866 4.155598 0.000000

22 6 0 2.186178 3.634616 0.000000

23 6 0 2.069289 2.192689 0.000000

24 7 0 3.121432 1.315579 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.480428 -5.581522 0.000000

27 1 0 -3.118657 -4.181859 0.000000

28 6 0 5.588584 -0.486053 0.000000

29 1 0 4.197333 -3.122439 0.000000

30 6 0 -5.588584 0.486053 0.000000

31 1 0 -4.197333 3.122439 0.000000

32 6 0 0.480428 5.581522 0.000000

33 1 0 3.118657 4.181859 0.000000

34 1 0 -1.339721 -6.254612 0.000000

35 1 0 0.133939 -5.809816 0.877893

36 1 0 0.133939 -5.809816 -0.877893

37 1 0 5.800199 0.133742 0.877681

38 1 0 5.800199 0.133742 -0.877681

39 1 0 6.274388 -1.334708 0.000000

40 1 0 -5.800199 -0.133742 0.877681

41 1 0 -5.800199 -0.133742 -0.877681

42 1 0 -6.274388 1.334708 0.000000

43 1 0 -0.133939 5.809816 0.877893

44 1 0 -0.133939 5.809816 -0.877893

45 1 0 1.339721 6.254612 0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.365439 0.000000

3 C 2.220762 1.358531 0.000000

4 C 2.278229 2.294640 1.465808 0.000000

5 C 1.446657 2.281623 2.271799 1.375771 0.000000

6 N 3.546464 2.438709 1.364225 2.501493 3.583067

7 C 4.253639 2.933119 2.376501 3.730748 4.639470

8 N 4.186803 2.834176 2.929991 4.395624 4.971738

9 C 5.524321 4.184399 4.251582 5.710251 6.334804

10 C 6.366888 5.002968 4.660710 6.019100 6.907690

11 C 5.728116 4.413447 3.752876 4.978476 6.022177

12 N 1.369791 2.441375 3.547344 3.597704 2.500527

13 C 3.768878 4.428339 5.737296 6.044592 4.982515

14 C 4.656944 4.991804 6.349129 6.909282 6.002646

15 C 4.267458 4.195191 5.527564 6.356973 5.707879

16 N 2.944244 2.839632 4.184510 4.990124 4.390859

17 C 2.378592 2.926568 4.242281 4.646914 3.721022

18 N 5.345968 5.010753 6.260411 7.274906 6.791048

19 N 4.938940 4.019419 4.930418 6.246370 6.233112

20 C 5.596844 4.930418 6.012781 7.220306 6.992519

21 C 7.013843 6.246370 7.220306 8.509364 8.384003

22 C 7.215711 6.233112 6.992519 8.384003 8.482879

23 C 6.029873 4.938940 5.596844 7.013843 7.215711

24 N 6.265104 5.006569 5.333038 6.797745 7.257766

25 Zn 3.014937 2.009709 3.006390 4.254682 4.241440

26 C 3.742816 3.723566 2.619022 1.490054 2.588441

27 H 2.248993 3.316663 3.330051 2.205947 1.081199

28 C 7.845739 6.480678 6.133316 7.465548 8.388109

29 H 6.335218 5.097491 4.201906 5.213593 6.404025

30 C 4.422792 5.386623 6.587581 6.588418 5.343807

31 H 5.725308 6.068600 7.426655 7.984832 7.050002

32 C 8.181650 7.548596 8.601504 9.836298 9.594164

33 H 8.218859 7.176737 7.836802 9.261014 9.446617

34 H 4.126923 4.427739 3.512529 2.141977 2.753338

35 H 4.325335 4.133278 2.940858 2.145445 3.299263

36 H 4.325335 4.133278 2.940858 2.145445 3.299263

37 H 8.252966 6.898576 6.656389 8.014612 8.874293

38 H 8.252966 6.898576 6.656389 8.014612 8.874293

39 H 8.387674 7.037766 6.496132 7.721013 8.767597

40 H 4.350779 5.417431 6.529188 6.389967 5.107601

41 H 4.350779 5.417431 6.529188 6.389967 5.107601

42 H 5.488659 6.391125 7.627306 7.673941 6.434876

43 H 8.279877 7.751069 8.860774 10.034286 9.704622

44 H 8.279877 7.751069 8.860774 10.034286 9.704622

45 H 9.109239 8.384691 9.357829 10.651132 10.498990

6 7 8 9 10

6 N 0.000000

7 C 1.321595 0.000000

8 N 2.414282 1.368096 0.000000

9 C 3.516259 2.231788 1.363935 0.000000

10 C 3.554347 2.292080 2.321109 1.501887 0.000000

11 C 2.478691 1.480340 2.305407 2.285312 1.350909

12 N 4.823545 5.357949 5.013025 6.261646 7.303498

13 C 6.848775 7.030884 6.260405 7.232045 8.551259

14 C 7.290537 7.228575 6.246764 7.006585 8.429461

15 C 6.273390 6.020789 4.926608 5.580341 7.030884

16 N 5.016626 4.926608 4.004549 4.914674 6.260405

17 C 5.348751 5.580341 4.914674 5.999355 7.232045

18 N 6.778951 6.273390 5.016626 5.348751 6.848775

19 N 5.010753 4.195191 2.839632 2.926568 4.428339

20 C 6.260411 5.527564 4.184510 4.242281 5.737296

21 C 7.274906 6.356973 4.990124 4.646914 6.044592

22 C 6.791048 5.707879 4.390859 3.721022 4.982515

23 C 5.345968 4.267458 2.944244 2.378592 3.768878

24 N 4.760113 3.516463 2.415774 1.317610 2.483768

25 Zn 3.389475 3.010395 2.002274 2.999678 4.275629

26 C 3.083532 4.404542 5.373435 6.580637 6.575452

27 H 4.603837 5.705285 6.049363 7.412970 7.981094

28 C 4.976291 3.757587 3.738591 2.634808 1.485886

29 H 2.839746 2.271481 3.335428 3.347618 2.187583

30 C 7.819888 8.181841 7.548388 8.601799 9.863629

31 H 8.345501 8.227987 7.185233 7.843726 9.301126

32 C 8.731398 7.841770 6.474009 6.120437 7.489582

33 H 7.497313 6.324762 5.084423 4.179946 5.224183

34 H 4.146249 5.467261 6.371634 7.615488 7.660216

35 H 3.095218 4.350844 5.422951 6.540568 6.390744

36 H 3.095218 4.350844 5.422951 6.540568 6.390744

37 H 5.567825 4.327550 4.132144 2.937719 2.136142

38 H 5.567825 4.327550 4.132144 2.937719 2.136142

39 H 5.225979 4.157835 4.454818 3.537630 2.139906

40 H 7.799837 8.261859 7.733345 8.844602 10.042906

41 H 7.799837 8.261859 7.733345 8.844602 10.042906

42 H 8.829779 9.117902 8.394735 9.369102 10.690257

43 H 9.081955 8.263190 6.906157 6.655997 8.050193

44 H 9.081955 8.263190 6.906157 6.655997 8.050193

45 H 9.360329 8.370428 7.017872 6.467651 7.727429

11 12 13 14 15

11 C 0.000000

12 N 6.835716 0.000000

13 C 8.429461 2.483768 0.000000

14 C 8.522764 3.541175 1.350909 0.000000

15 C 7.228575 3.516463 2.292080 1.480340 0.000000

16 N 6.246764 2.415774 2.321109 2.305407 1.368096

17 C 7.006585 1.317610 1.501887 2.285312 2.231788

18 N 7.290537 4.760113 3.554347 2.478691 1.321595

19 N 4.991804 5.006569 5.002968 4.413447 2.933119

20 C 6.349129 5.333038 4.660710 3.752876 2.376501

21 C 6.909282 6.797745 6.019100 4.978476 3.730748

22 C 6.002646 7.257766 6.907690 6.022177 4.639470

23 C 4.656944 6.265104 6.366888 5.728116 4.253639

24 N 3.541175 6.774685 7.303498 6.835716 5.357949

25 Zn 4.261382 3.387342 4.275629 4.261382 3.010395

26 C 5.354677 5.017288 7.489582 8.391339 7.841770

27 H 7.065644 2.866282 5.224183 6.389317 6.324762

28 C 2.570796 8.749428 9.863629 9.625320 8.181841

29 H 1.081465 7.538506 9.301126 9.480698 8.227987

30 C 9.625320 3.054948 1.485886 2.570796 3.757587

31 H 9.480698 4.566570 2.187583 1.081465 2.271481

32 C 8.391339 7.780963 6.575452 5.354677 4.404542

33 H 6.389317 8.316282 7.981094 7.065644 5.705285

34 H 6.445972 5.250576 7.727429 8.752042 8.370428

35 H 5.132037 5.618390 8.050193 8.891915 8.263190

36 H 5.132037 5.618390 8.050193 8.891915 8.263190

37 H 3.275737 9.081099 10.042906 9.718505 8.261859

38 H 3.275737 9.081099 10.042906 9.718505 8.261859

39 H 2.750177 9.395839 10.690257 10.538218 9.117902

40 H 9.718505 3.056608 2.136142 3.275737 4.327550

41 H 9.718505 3.056608 2.136142 3.275737 4.327550

42 H 10.538218 4.118877 2.139906 2.750177 4.157835

43 H 8.891915 7.776057 6.390744 5.132037 4.350844

44 H 8.891915 7.776057 6.390744 5.132037 4.350844

45 H 8.752042 8.786904 7.660216 6.445972 5.467261

16 17 18 19 20

16 N 0.000000

17 C 1.363935 0.000000

18 N 2.414282 3.516259 0.000000

19 N 2.834176 4.184399 2.438709 0.000000

20 C 2.929991 4.251582 1.364225 1.358531 0.000000

21 C 4.395624 5.710251 2.501493 2.294640 1.465808

22 C 4.971738 6.334804 3.583067 2.281623 2.271799

23 C 4.186803 5.524321 3.546464 1.365439 2.220762

24 N 5.013025 6.261646 4.823545 2.441375 3.547344

25 Zn 2.002274 2.999678 3.389475 2.009709 3.006390

26 C 6.474009 6.120437 8.731398 7.548596 8.601504

27 H 5.084423 4.179946 7.497313 7.176737 7.836802

28 C 7.548388 8.601799 7.819888 5.386623 6.587581

29 H 7.185233 7.843726 8.345501 6.068600 7.426655

30 C 3.738591 2.634808 4.976291 6.480678 6.133316

31 H 3.335428 3.347618 2.839746 5.097491 4.201906

32 C 5.373435 6.580637 3.083532 3.723566 2.619022

33 H 6.049363 7.412970 4.603837 3.316663 3.330051

34 H 7.017872 6.467651 9.360329 8.384691 9.357829

35 H 6.906157 6.655997 9.081955 7.751069 8.860774

36 H 6.906157 6.655997 9.081955 7.751069 8.860774

37 H 7.733345 8.844602 7.799837 5.417431 6.529188

38 H 7.733345 8.844602 7.799837 5.417431 6.529188

39 H 8.394735 9.369102 8.829779 6.391125 7.627306

40 H 4.132144 2.937719 5.567825 6.898576 6.656389

41 H 4.132144 2.937719 5.567825 6.898576 6.656389

42 H 4.454818 3.537630 5.225979 7.037766 6.496132

43 H 5.422951 6.540568 3.095218 4.133278 2.940858

44 H 5.422951 6.540568 3.095218 4.133278 2.940858

45 H 6.371634 7.615488 4.146249 4.427739 3.512529

21 22 23 24 25

21 C 0.000000

22 C 1.375771 0.000000

23 C 2.278229 1.446657 0.000000

24 N 3.597704 2.500527 1.369791 0.000000

25 Zn 4.254682 4.241440 3.014937 3.387342 0.000000

26 C 9.836298 9.594164 8.181650 7.780963 5.602160

27 H 9.261014 9.446617 8.218859 8.316282 5.216701

28 C 6.588418 5.343807 4.422792 3.054948 5.609680

29 H 7.984832 7.050002 5.725308 4.566570 5.231369

30 C 7.465548 8.388109 7.845739 8.749428 5.609680

31 H 5.213593 6.404025 6.335218 7.538506 5.231369

32 C 1.490054 2.588441 3.742816 5.017288 5.602160

33 H 2.205947 1.081199 2.248993 2.866282 5.216701

34 H 10.651132 10.498990 9.109239 8.786904 6.396485

35 H 10.034286 9.704622 8.279877 7.776057 5.877295

36 H 10.034286 9.704622 8.279877 7.776057 5.877295

37 H 6.389967 5.107601 4.350779 3.056608 5.867753

38 H 6.389967 5.107601 4.350779 3.056608 5.867753

39 H 7.673941 6.434876 5.488659 4.118877 6.414779

40 H 8.014612 8.874293 8.252966 9.081099 5.867753

41 H 8.014612 8.874293 8.252966 9.081099 5.867753

42 H 7.721013 8.767597 8.387674 9.395839 6.414779

43 H 2.145445 3.299263 4.325335 5.618390 5.877295

44 H 2.145445 3.299263 4.325335 5.618390 5.877295

45 H 2.141977 2.753338 4.126923 5.250576 6.396485

26 27 28 29 30

26 C 0.000000

27 H 2.986521 0.000000

28 C 7.924437 9.459124 0.000000

29 H 5.284745 7.392299 2.980958 0.000000

30 C 7.931501 5.281092 11.219361 10.430022 0.000000

31 H 9.464370 7.383516 10.430022 10.462739 2.980958

32 C 11.204319 10.405624 7.931501 9.464370 7.924437

33 H 10.405624 10.433402 5.281092 7.383516 9.459124

34 H 1.091529 2.731468 9.015413 6.361562 7.968023

35 H 1.095564 3.741700 7.672438 4.950138 8.553124

36 H 1.095564 3.741700 7.672438 4.950138 8.553124

37 H 8.537027 9.946896 1.095103 3.733928 11.427984

38 H 8.537027 9.946896 1.095103 3.733928 11.427984

39 H 7.978907 9.815068 1.091120 2.740463 12.001885

40 H 7.664763 4.934394 11.427984 10.471546 1.095103

41 H 7.664763 4.934394 11.427984 10.471546 1.095103

42 H 9.022428 6.355403 12.001885 11.380821 1.091120

43 H 11.430368 10.464837 8.553124 9.965731 7.672438

44 H 11.430368 10.464837 8.553124 9.965731 7.672438

45 H 11.975266 11.348879 7.968023 9.802807 9.015413

31 32 33 34 35

31 H 0.000000

32 C 5.284745 0.000000

33 H 7.392299 2.986521 0.000000

34 H 9.802807 11.975266 11.348879 0.000000

35 H 9.965731 11.430368 10.464837 1.772065 0.000000

36 H 9.965731 11.430368 10.464837 1.772065 1.755786

37 H 10.471546 7.664763 4.934394 9.620803 8.211722

38 H 10.471546 7.664763 4.934394 9.620803 8.397287

39 H 11.380821 9.022428 6.355403 9.065324 7.648686

40 H 3.733928 8.537027 9.946896 7.624385 8.211688

41 H 3.733928 8.537027 9.946896 7.624385 8.397253

42 H 2.740463 7.978907 9.815068 9.052553 9.637508

43 H 4.950138 1.095564 3.741700 12.156275 11.622720

44 H 4.950138 1.095564 3.741700 12.156275 11.754590

45 H 6.361562 1.091529 2.731468 12.792970 12.156275

36 37 38 39 40

36 H 0.000000

37 H 8.397287 0.000000

38 H 8.211722 1.755363 0.000000

39 H 7.648686 1.775253 1.775253 0.000000

40 H 8.397253 11.603482 11.735505 12.165866 0.000000

41 H 8.211688 11.735505 11.603482 12.165866 1.755363

42 H 9.637508 12.165866 12.165866 12.829557 1.775253

43 H 11.754590 8.211688 8.397253 9.637508 8.211722

44 H 11.622720 8.397253 8.211688 9.637508 8.397287

45 H 12.156275 7.624385 7.624385 9.052553 9.620803

41 42 43 44 45

41 H 0.000000

42 H 1.775253 0.000000

43 H 8.397287 7.648686 0.000000

44 H 8.211722 7.648686 1.755786 0.000000

45 H 9.620803 9.065324 1.772065 1.772065 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=0 Diff= 3.11D-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 2.943456 -0.652616 0.000000

2 7 0 1.984211 0.319121 0.000000

3 6 0 2.582807 1.538665 0.000000

4 6 0 4.035973 1.346567 0.000000

5 6 0 4.241417 -0.013778 0.000000

6 7 0 1.970565 2.757792 0.000000

7 6 0 0.661162 2.936893 0.000000

8 7 0 -0.314138 1.977478 0.000000

9 6 0 -1.540871 2.573671 0.000000

10 6 0 -1.336044 4.061526 0.000000

11 6 0 0.000000 4.261382 0.000000

12 7 0 2.729748 -2.005634 0.000000

13 6 0 1.336044 -4.061526 0.000000

14 6 0 -0.000000 -4.261382 0.000000

15 6 0 -0.661162 -2.936893 0.000000

16 7 0 0.314138 -1.977478 0.000000

17 6 0 1.540871 -2.573671 0.000000

18 7 0 -1.970565 -2.757792 0.000000

19 7 0 -1.984211 -0.319121 0.000000

20 6 0 -2.582807 -1.538665 0.000000

21 6 0 -4.035973 -1.346567 0.000000

22 6 0 -4.241417 0.013778 0.000000

23 6 0 -2.943456 0.652616 0.000000

24 7 0 -2.729748 2.005634 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 5.038582 2.448854 0.000000

27 1 0 5.189312 -0.533862 0.000000

28 6 0 -2.447644 5.047529 0.000000

29 1 0 0.529176 5.204536 0.000000

30 6 0 2.447644 -5.047529 0.000000

31 1 0 -0.529176 -5.204536 0.000000

32 6 0 -5.038582 -2.448854 0.000000

33 1 0 -5.189312 0.533862 0.000000

34 1 0 6.057011 2.056123 0.000000

35 1 0 4.919643 3.093383 0.877893

36 1 0 4.919643 3.093383 -0.877893

37 1 0 -3.088284 4.911487 0.877681

38 1 0 -3.088284 4.911487 -0.877681

39 1 0 -2.070564 6.071421 0.000000

40 1 0 3.088284 -4.911487 0.877681

41 1 0 3.088284 -4.911487 -0.877681

42 1 0 2.070564 -6.071421 0.000000

43 1 0 -4.919643 -3.093383 0.877893

44 1 0 -4.919643 -3.093383 -0.877893

45 1 0 -6.057011 -2.056123 0.000000

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

Rotational constants (GHZ): 0.1828384 0.1816680 0.0913302

Leave Link 202 at Tue Sep 17 14:32:55 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 101 beta electrons

nuclear repulsion energy 2760.6583259399 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= -0.1141671093 Hartrees.

Nuclear repulsion after empirical dispersion term = 2760.5441588305 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 = 0.48D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 242

GePol: Fraction of low-weight points (<1% of avg) = 6.73%

GePol: Cavity surface area = 378.813 Ang\*\*2

GePol: Cavity volume = 378.348 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0106823351 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2760.5334764955 Hartrees.

Leave Link 301 at Tue Sep 17 14:32:55 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= 15323 LenP2D= 41242.

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 14:32:56 2019, MaxMem= 2415919104 cpu: 14.1

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:32:56 2019, MaxMem= 2415919104 cpu: 1.7

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= -0.000000 -0.000000 0.000000

Rot= 0.993896 -0.000000 -0.000000 0.110325 Ang= 12.67 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 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0181 S= 1.0060

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= -1276.14820954681

Leave Link 401 at Tue Sep 17 14:32:58 2019, MaxMem= 2415919104 cpu: 43.0

(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 1.24D-14 for 3582.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.66D-15 for 3595 1330.

Iteration 1 A^-1\*A deviation from unit magnitude is 1.24D-14 for 3582.

Iteration 1 A^-1\*A deviation from orthogonality is 3.41D-11 for 1666 1644.

E= -1275.84167936648

DIIS: error= 7.88D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.84167936648 IErMin= 1 ErrMin= 7.88D-04

ErrMax= 7.88D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.41D-03 BMatP= 2.41D-03

IDIUse=3 WtCom= 9.92D-01 WtEn= 7.88D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.304 Goal= None Shift= 0.000

Gap= 0.393 Goal= None Shift= 0.000

RMSDP=7.65D-05 MaxDP=1.92D-03 OVMax= 1.54D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 7.65D-05 CP: 1.00D+00

E= -1275.84257285103 Delta-E= -0.000893484549 Rises=F Damp=F

DIIS: error= 4.22D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84257285103 IErMin= 2 ErrMin= 4.22D-04

ErrMax= 4.22D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.00D-04 BMatP= 2.41D-03

IDIUse=3 WtCom= 9.96D-01 WtEn= 4.22D-03

Coeff-Com: 0.718D-01 0.928D+00

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

Coeff: 0.715D-01 0.928D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=3.06D-05 MaxDP=1.32D-03 DE=-8.93D-04 OVMax= 1.76D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.04D-05 CP: 1.00D+00 1.05D+00

E= -1275.84254822307 Delta-E= 0.000024627962 Rises=F Damp=F

DIIS: error= 7.37D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1275.84257285103 IErMin= 2 ErrMin= 4.22D-04

ErrMax= 7.37D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.86D-04 BMatP= 2.00D-04

IDIUse=3 WtCom= 2.69D-01 WtEn= 7.31D-01

Coeff-Com: -0.293D-01 0.631D+00 0.399D+00

Coeff-En: 0.000D+00 0.579D+00 0.421D+00

Coeff: -0.788D-02 0.593D+00 0.415D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=1.74D-05 MaxDP=7.16D-04 DE= 2.46D-05 OVMax= 3.37D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.33D-05 CP: 1.00D+00 1.12D+00 6.66D-01

E= -1275.84265651546 Delta-E= -0.000108292392 Rises=F Damp=F

DIIS: error= 2.30D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84265651546 IErMin= 4 ErrMin= 2.30D-04

ErrMax= 2.30D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.36D-05 BMatP= 2.00D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.30D-03

Coeff-Com: -0.116D-01 0.168D+00 0.174D+00 0.669D+00

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

Coeff: -0.116D-01 0.168D+00 0.173D+00 0.670D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=9.94D-06 MaxDP=5.20D-04 DE=-1.08D-04 OVMax= 7.16D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.94D-06 CP: 1.00D+00 1.14D+00 9.23D-01 1.23D+00

E= -1275.84266955209 Delta-E= -0.000013036626 Rises=F Damp=F

DIIS: error= 1.67D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84266955209 IErMin= 5 ErrMin= 1.67D-04

ErrMax= 1.67D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.70D-06 BMatP= 1.36D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.67D-03

Coeff-Com: -0.237D-03-0.360D-01-0.631D-03 0.470D+00 0.567D+00

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

Coeff: -0.237D-03-0.359D-01-0.630D-03 0.469D+00 0.568D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=7.72D-06 MaxDP=3.39D-04 DE=-1.30D-05 OVMax= 5.60D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.10D-06 CP: 1.00D+00 1.17D+00 1.07D+00 1.64D+00 1.19D+00

E= -1275.84267919744 Delta-E= -0.000009645356 Rises=F Damp=F

DIIS: error= 1.32D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84267919744 IErMin= 6 ErrMin= 1.32D-04

ErrMax= 1.32D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.08D-06 BMatP= 8.70D-06

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.32D-03

Coeff-Com: 0.969D-02-0.133D+00-0.175D+00-0.315D+00-0.837D-01 0.170D+01

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

Coeff: 0.968D-02-0.132D+00-0.174D+00-0.314D+00-0.835D-01 0.169D+01

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=1.93D-05 MaxDP=9.65D-04 DE=-9.65D-06 OVMax= 1.48D-02

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.12D-06 CP: 1.00D+00 1.25D+00 1.47D+00 2.55D+00 2.39D+00

CP: 2.68D+00

E= -1275.84269423363 Delta-E= -0.000015036191 Rises=F Damp=F

DIIS: error= 7.88D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84269423363 IErMin= 7 ErrMin= 7.88D-05

ErrMax= 7.88D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.38D-06 BMatP= 3.08D-06

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

Coeff-Com: 0.792D-02-0.810D-01-0.153D+00-0.508D+00-0.432D+00 0.142D+01

Coeff-Com: 0.747D+00

Coeff: 0.792D-02-0.810D-01-0.153D+00-0.508D+00-0.432D+00 0.142D+01

Coeff: 0.747D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=1.40D-05 MaxDP=6.85D-04 DE=-1.50D-05 OVMax= 1.06D-02

Cycle 8 Pass 1 IDiag 1:

RMSU= 4.10D-06 CP: 1.00D+00 1.29D+00 1.76D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.37D+00

E= -1275.84269986095 Delta-E= -0.000005627317 Rises=F Damp=F

DIIS: error= 2.88D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84269986095 IErMin= 8 ErrMin= 2.88D-05

ErrMax= 2.88D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.55D-07 BMatP= 2.38D-06

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

Coeff-Com: -0.178D-02 0.427D-01 0.204D-01-0.129D-01-0.996D-01-0.241D+00

Coeff-Com: 0.233D+00 0.106D+01

Coeff: -0.178D-02 0.427D-01 0.204D-01-0.129D-01-0.996D-01-0.241D+00

Coeff: 0.233D+00 0.106D+01

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=6.13D-06 MaxDP=3.23D-04 DE=-5.63D-06 OVMax= 4.73D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.92D-06 CP: 1.00D+00 1.31D+00 1.87D+00 3.00D+00 3.00D+00

CP: 3.00D+00 1.87D+00 2.02D+00

E= -1275.84270086837 Delta-E= -0.000001007417 Rises=F Damp=F

DIIS: error= 1.32D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84270086837 IErMin= 9 ErrMin= 1.32D-05

ErrMax= 1.32D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.63D-07 BMatP= 3.55D-07

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

Coeff-Com: -0.233D-02 0.372D-01 0.354D-01 0.829D-01 0.351D-01-0.372D+00

Coeff-Com: -0.383D-01 0.593D+00 0.629D+00

Coeff: -0.233D-02 0.372D-01 0.354D-01 0.829D-01 0.351D-01-0.372D+00

Coeff: -0.383D-01 0.593D+00 0.629D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=1.32D-06 MaxDP=7.15D-05 DE=-1.01D-06 OVMax= 9.51D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 4.39D-07 CP: 1.00D+00 1.32D+00 1.90D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.04D+00 2.25D+00 1.13D+00

E= -1275.84270100977 Delta-E= -0.000000141404 Rises=F Damp=F

DIIS: error= 6.40D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84270100977 IErMin=10 ErrMin= 6.40D-06

ErrMax= 6.40D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.90D-08 BMatP= 1.63D-07

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

Coeff-Com: -0.302D-03-0.180D-02 0.584D-02 0.465D-01 0.670D-01-0.603D-01

Coeff-Com: -0.159D+00-0.164D+00 0.295D+00 0.971D+00

Coeff: -0.302D-03-0.180D-02 0.584D-02 0.465D-01 0.670D-01-0.603D-01

Coeff: -0.159D+00-0.164D+00 0.295D+00 0.971D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=1.05D-06 MaxDP=5.88D-05 DE=-1.41D-07 OVMax= 7.53D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 3.47D-07 CP: 1.00D+00 1.32D+00 1.91D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.18D+00 2.42D+00 1.25D+00 1.47D+00

E= -1275.84270107625 Delta-E= -0.000000066480 Rises=F Damp=F

DIIS: error= 4.33D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84270107625 IErMin=11 ErrMin= 4.33D-06

ErrMax= 4.33D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.03D-08 BMatP= 3.90D-08

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

Coeff-Com: 0.281D-03-0.734D-02-0.443D-02 0.788D-02 0.183D-01 0.488D-01

Coeff-Com: -0.772D-01-0.159D+00 0.172D-02 0.391D+00 0.780D+00

Coeff: 0.281D-03-0.734D-02-0.443D-02 0.788D-02 0.183D-01 0.488D-01

Coeff: -0.772D-01-0.159D+00 0.172D-02 0.391D+00 0.780D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=3.87D-07 MaxDP=2.09D-05 DE=-6.65D-08 OVMax= 2.68D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.16D-07 CP: 1.00D+00 1.32D+00 1.92D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.23D+00 2.48D+00 1.29D+00 1.72D+00

CP: 1.31D+00

E= -1275.84270108914 Delta-E= -0.000000012894 Rises=F Damp=F

DIIS: error= 2.30D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84270108914 IErMin=12 ErrMin= 2.30D-06

ErrMax= 2.30D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.93D-09 BMatP= 1.03D-08

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

Coeff-Com: 0.264D-03-0.349D-02-0.528D-02-0.129D-01-0.198D-01 0.536D-01

Coeff-Com: 0.842D-02-0.117D-01-0.115D+00-0.172D+00 0.457D+00 0.821D+00

Coeff: 0.264D-03-0.349D-02-0.528D-02-0.129D-01-0.198D-01 0.536D-01

Coeff: 0.842D-02-0.117D-01-0.115D+00-0.172D+00 0.457D+00 0.821D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=4.22D-07 MaxDP=2.20D-05 DE=-1.29D-08 OVMax= 3.21D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 8.62D-08 CP: 1.00D+00 1.32D+00 1.93D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.26D+00 2.54D+00 1.36D+00 1.87D+00

CP: 1.48D+00 1.35D+00

E= -1275.84270109564 Delta-E= -0.000000006492 Rises=F Damp=F

DIIS: error= 8.78D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84270109564 IErMin=13 ErrMin= 8.78D-07

ErrMax= 8.78D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.03D-10 BMatP= 4.93D-09

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

Coeff-Com: 0.466D-04 0.420D-03-0.117D-02-0.670D-02-0.139D-01 0.108D-01

Coeff-Com: 0.175D-01 0.388D-01-0.563D-01-0.180D+00 0.351D-01 0.385D+00

Coeff-Com: 0.770D+00

Coeff: 0.466D-04 0.420D-03-0.117D-02-0.670D-02-0.139D-01 0.108D-01

Coeff: 0.175D-01 0.388D-01-0.563D-01-0.180D+00 0.351D-01 0.385D+00

Coeff: 0.770D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=2.07D-07 MaxDP=1.09D-05 DE=-6.49D-09 OVMax= 1.58D-04

Cycle 14 Pass 1 IDiag 1:

RMSU= 3.44D-08 CP: 1.00D+00 1.32D+00 1.93D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.27D+00 2.58D+00 1.39D+00 1.92D+00

CP: 1.54D+00 1.65D+00 1.29D+00

E= -1275.84270109672 Delta-E= -0.000000001089 Rises=F Damp=F

DIIS: error= 4.95D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84270109672 IErMin=14 ErrMin= 4.95D-07

ErrMax= 4.95D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.60D-10 BMatP= 8.03D-10

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

Coeff-Com: -0.247D-04 0.101D-02 0.382D-03-0.142D-02-0.422D-02-0.529D-02

Coeff-Com: 0.915D-02 0.297D-01-0.814D-02-0.743D-01-0.898D-01 0.458D-01

Coeff-Com: 0.466D+00 0.631D+00

Coeff: -0.247D-04 0.101D-02 0.382D-03-0.142D-02-0.422D-02-0.529D-02

Coeff: 0.915D-02 0.297D-01-0.814D-02-0.743D-01-0.898D-01 0.458D-01

Coeff: 0.466D+00 0.631D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=5.48D-08 MaxDP=2.72D-06 DE=-1.09D-09 OVMax= 4.00D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 1.42D-08 CP: 1.00D+00 1.32D+00 1.93D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.27D+00 2.58D+00 1.39D+00 1.94D+00

CP: 1.55D+00 1.74D+00 1.46D+00 9.96D-01

E= -1275.84270109684 Delta-E= -0.000000000117 Rises=F Damp=F

DIIS: error= 1.64D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.84270109684 IErMin=15 ErrMin= 1.64D-07

ErrMax= 1.64D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.24D-11 BMatP= 2.60D-10

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

Coeff-Com: -0.193D-04 0.327D-03 0.385D-03 0.692D-03 0.115D-02-0.415D-02

Coeff-Com: 0.335D-03 0.399D-02 0.659D-02 0.348D-02-0.437D-01-0.481D-01

Coeff-Com: 0.367D-01 0.273D+00 0.769D+00

Coeff: -0.193D-04 0.327D-03 0.385D-03 0.692D-03 0.115D-02-0.415D-02

Coeff: 0.335D-03 0.399D-02 0.659D-02 0.348D-02-0.437D-01-0.481D-01

Coeff: 0.367D-01 0.273D+00 0.769D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=1.10D-08 MaxDP=6.17D-07 DE=-1.17D-10 OVMax= 4.11D-06

Cycle 16 Pass 1 IDiag 1:

RMSU= 7.13D-09 CP: 1.00D+00 1.32D+00 1.93D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.27D+00 2.58D+00 1.39D+00 1.94D+00

CP: 1.56D+00 1.78D+00 1.50D+00 1.09D+00 1.15D+00

E= -1275.84270109688 Delta-E= -0.000000000035 Rises=F Damp=F

DIIS: error= 8.23D-08 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1275.84270109688 IErMin=16 ErrMin= 8.23D-08

ErrMax= 8.23D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.71D-12 BMatP= 3.24D-11

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

Coeff-Com: -0.603D-05-0.441D-04 0.148D-03 0.782D-03 0.170D-02-0.117D-02

Coeff-Com: -0.196D-02-0.481D-02 0.589D-02 0.191D-01-0.318D-02-0.355D-01

Coeff-Com: -0.817D-01 0.149D-01 0.403D+00 0.683D+00

Coeff: -0.603D-05-0.441D-04 0.148D-03 0.782D-03 0.170D-02-0.117D-02

Coeff: -0.196D-02-0.481D-02 0.589D-02 0.191D-01-0.318D-02-0.355D-01

Coeff: -0.817D-01 0.149D-01 0.403D+00 0.683D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=1.03D-08 MaxDP=5.52D-07 DE=-3.50D-11 OVMax= 7.03D-06

Cycle 17 Pass 1 IDiag 1:

RMSU= 3.68D-09 CP: 1.00D+00 1.32D+00 1.93D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.27D+00 2.58D+00 1.39D+00 1.94D+00

CP: 1.57D+00 1.78D+00 1.51D+00 1.12D+00 1.32D+00

CP: 1.23D+00

E= -1275.84270109686 Delta-E= 0.000000000012 Rises=F Damp=F

DIIS: error= 5.35D-08 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=16 EnMin= -1275.84270109688 IErMin=17 ErrMin= 5.35D-08

ErrMax= 5.35D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.09D-12 BMatP= 9.71D-12

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

Coeff-Com: 0.158D-05-0.103D-03-0.172D-04 0.194D-03 0.578D-03 0.490D-03

Coeff-Com: -0.931D-03-0.350D-02 0.184D-02 0.888D-02 0.834D-02-0.886D-02

Coeff-Com: -0.510D-01-0.591D-01 0.292D-01 0.404D+00 0.670D+00

Coeff: 0.158D-05-0.103D-03-0.172D-04 0.194D-03 0.578D-03 0.490D-03

Coeff: -0.931D-03-0.350D-02 0.184D-02 0.888D-02 0.834D-02-0.886D-02

Coeff: -0.510D-01-0.591D-01 0.292D-01 0.404D+00 0.670D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=5.77D-09 MaxDP=3.08D-07 DE= 1.23D-11 OVMax= 4.08D-06

Error on total polarization charges = 0.06477

SCF Done: E(UB3LYP) = -1275.84270110 A.U. after 17 cycles

NFock= 17 Conv=0.58D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0177 S= 1.0059

<L.S>= 0.000000000000E+00

KE= 1.320772539022D+03 PE=-8.573018550899D+03 EE= 3.215869834284D+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 2.0177, after 2.0002

Leave Link 502 at Tue Sep 17 14:34:27 2019, MaxMem= 2415919104 cpu: 1562.6

(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= 41242.

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 14:34:31 2019, MaxMem= 2415919104 cpu: 69.2

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 14:34:31 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 14:34:41 2019, MaxMem= 2415919104 cpu: 177.5

(Enter /home/blab/g09/l716.exe)

Dipole =-3.28626015D-13 2.05613304D-13 6.66133815D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000172496 0.000363113 -0.000000000

2 7 0.000153893 0.000297686 0.000000000

3 6 0.000029097 0.002047937 0.000000000

4 6 -0.001197072 -0.000735502 -0.000000000

5 6 0.000805886 -0.000177578 -0.000000000

6 7 0.000832679 -0.000710330 -0.000000000

7 6 -0.001783039 0.000035404 -0.000000000

8 7 -0.000213761 -0.000032060 0.000000000

9 6 -0.001281725 0.001941820 0.000000000

10 6 0.000238798 -0.001785314 0.000000000

11 6 0.000882063 0.001127424 -0.000000000

12 7 -0.000261072 0.000226089 0.000000000

13 6 -0.000238798 0.001785314 0.000000000

14 6 -0.000882063 -0.001127424 0.000000000

15 6 0.001783039 -0.000035404 0.000000000

16 7 0.000213761 0.000032060 0.000000000

17 6 0.001281725 -0.001941820 -0.000000000

18 7 -0.000832679 0.000710330 -0.000000000

19 7 -0.000153893 -0.000297686 -0.000000000

20 6 -0.000029097 -0.002047937 0.000000000

21 6 0.001197072 0.000735502 -0.000000000

22 6 -0.000805886 0.000177578 0.000000000

23 6 0.000172496 -0.000363113 0.000000000

24 7 0.000261072 -0.000226089 -0.000000000

25 30 0.000000000 0.000000000 -0.000000000

26 6 0.000036099 0.000455067 0.000000000

27 1 0.000009578 0.000158573 0.000000000

28 6 -0.000247863 0.000245690 -0.000000000

29 1 -0.000280851 0.000107317 -0.000000000

30 6 0.000247863 -0.000245690 -0.000000000

31 1 0.000280851 -0.000107317 -0.000000000

32 6 -0.000036099 -0.000455067 -0.000000000

33 1 -0.000009578 -0.000158573 -0.000000000

34 1 0.000155730 -0.000009185 -0.000000000

35 1 -0.000111843 0.000126519 -0.000286867

36 1 -0.000111843 0.000126519 0.000286867

37 1 -0.000043295 -0.000053534 -0.000265954

38 1 -0.000043295 -0.000053534 0.000265954

39 1 -0.000014715 0.000163107 -0.000000000

40 1 0.000043295 0.000053534 -0.000265954

41 1 0.000043295 0.000053534 0.000265954

42 1 0.000014715 -0.000163107 -0.000000000

43 1 0.000111843 -0.000126519 -0.000286867

44 1 0.000111843 -0.000126519 0.000286867

45 1 -0.000155730 0.000009185 -0.000000000

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

Cartesian Forces: Max 0.002047937 RMS 0.000586826

Leave Link 716 at Tue Sep 17 14:34:41 2019, MaxMem= 2415919104 cpu: 0.4

(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 0.001445493 RMS 0.000327265

Search for a local minimum.

Step number 26 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 12 13 14 15

16 17 18 19 20

21 22 23 24 25

26

DE= 1.28D-03 DEPred=-6.64D-04 R=-1.93D+00

Trust test=-1.93D+00 RLast= 8.50D-02 DXMaxT set to 5.00D-02

ITU= -1 1 -1 -1 1 0 0 1 -1 -1 1 1 -1 1 1 1 -1 0 1 -1

ITU= 1 1 1 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01335

Eigenvalues --- 0.01336 0.01343 0.01344 0.01604 0.01623

Eigenvalues --- 0.01631 0.01640 0.01774 0.01792 0.01808

Eigenvalues --- 0.01821 0.01888 0.01908 0.01939 0.01949

Eigenvalues --- 0.01997 0.01999 0.02044 0.02047 0.02070

Eigenvalues --- 0.02087 0.02102 0.02110 0.02114 0.02205

Eigenvalues --- 0.02313 0.02316 0.02351 0.02373 0.06263

Eigenvalues --- 0.07173 0.07211 0.07211 0.07213 0.07213

Eigenvalues --- 0.07302 0.07389 0.07752 0.09694 0.11887

Eigenvalues --- 0.14314 0.14496 0.14500 0.15684 0.15804

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16008 0.16164 0.16723 0.17426 0.19070

Eigenvalues --- 0.22061 0.22093 0.22158 0.22562 0.23842

Eigenvalues --- 0.23855 0.23894 0.24154 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25328

Eigenvalues --- 0.25371 0.27374 0.29000 0.31561 0.32663

Eigenvalues --- 0.33191 0.33196 0.33282 0.33282 0.33678

Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33747 0.34159 0.34437 0.34437

Eigenvalues --- 0.34438 0.34443 0.35035 0.35554 0.35565

Eigenvalues --- 0.35682 0.35682 0.35690 0.35785 0.37223

Eigenvalues --- 0.38390 0.41643 0.41819 0.42863 0.46469

Eigenvalues --- 0.46950 0.48965 0.48982 0.50952 0.51348

Eigenvalues --- 0.51359 0.51361 0.53928 0.54015 0.54022

Eigenvalues --- 0.54610 0.56324 0.56330 0.70586

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 1.16730 -0.19576 -0.17437 0.20284

Cosine: 0.983 > 0.710

Length: 1.080

GDIIS step was calculated using 4 of the last 26 vectors.

Iteration 1 RMS(Cart)= 0.00394157 RMS(Int)= 0.00000537

Iteration 2 RMS(Cart)= 0.00000955 RMS(Int)= 0.00000148

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000148

ITry= 1 IFail=0 DXMaxC= 1.47D-02 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 3.51D-10 for atom 27.

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

(Linear) (Quad) (Total)

R1 2.58031 -0.00014 -0.00144 0.00087 -0.00057 2.57974

R2 2.73379 -0.00029 0.00092 -0.00066 0.00025 2.73404

R3 2.58853 -0.00088 0.00049 -0.00196 -0.00147 2.58705

R4 2.56725 -0.00093 -0.00064 -0.00289 -0.00352 2.56373

R5 3.79780 -0.00103 -0.00018 -0.00068 -0.00086 3.79694

R6 2.76998 0.00047 0.00258 0.00075 0.00333 2.77331

R7 2.57801 0.00010 0.00080 0.00009 0.00089 2.57890

R8 2.59983 -0.00096 -0.00172 -0.00074 -0.00246 2.59737

R9 2.81579 -0.00068 -0.00100 -0.00165 -0.00265 2.81314

R10 2.04317 -0.00009 0.00004 -0.00007 -0.00003 2.04314

R11 2.49745 -0.00052 -0.00192 0.00225 0.00033 2.49778

R12 2.58533 -0.00039 0.00099 -0.00236 -0.00138 2.58395

R13 2.79744 0.00039 0.00190 -0.00042 0.00149 2.79892

R14 2.57746 -0.00016 -0.00221 0.00121 -0.00100 2.57647

R15 3.78375 -0.00145 -0.00110 -0.00310 -0.00420 3.77955

R16 2.83816 0.00034 0.00457 -0.00239 0.00219 2.84034

R17 2.48992 -0.00099 -0.00097 0.00092 -0.00004 2.48988

R18 2.55285 -0.00104 -0.00203 -0.00039 -0.00243 2.55042

R19 2.80792 -0.00024 -0.00080 0.00044 -0.00037 2.80755

R20 2.04367 -0.00023 -0.00018 -0.00010 -0.00028 2.04340

R21 2.48992 -0.00099 -0.00097 0.00092 -0.00004 2.48988

R22 2.55285 -0.00104 -0.00203 -0.00039 -0.00243 2.55042

R23 2.83816 0.00034 0.00457 -0.00239 0.00219 2.84034

R24 2.80792 -0.00024 -0.00080 0.00044 -0.00037 2.80755

R25 2.79744 0.00039 0.00190 -0.00042 0.00149 2.79892

R26 2.04367 -0.00023 -0.00018 -0.00010 -0.00028 2.04340

R27 2.58533 -0.00039 0.00099 -0.00236 -0.00138 2.58395

R28 2.49745 -0.00052 -0.00192 0.00225 0.00033 2.49778

R29 2.57746 -0.00016 -0.00221 0.00121 -0.00100 2.57647

R30 3.78375 -0.00145 -0.00110 -0.00310 -0.00420 3.77955

R31 2.57801 0.00010 0.00080 0.00009 0.00089 2.57890

R32 2.56725 -0.00093 -0.00064 -0.00289 -0.00352 2.56373

R33 2.58031 -0.00014 -0.00144 0.00087 -0.00057 2.57974

R34 3.79780 -0.00103 -0.00018 -0.00068 -0.00086 3.79694

R35 2.76998 0.00047 0.00258 0.00075 0.00333 2.77331

R36 2.59983 -0.00096 -0.00172 -0.00074 -0.00246 2.59737

R37 2.81579 -0.00068 -0.00100 -0.00165 -0.00265 2.81314

R38 2.73379 -0.00029 0.00092 -0.00066 0.00025 2.73404

R39 2.04317 -0.00009 0.00004 -0.00007 -0.00003 2.04314

R40 2.58853 -0.00088 0.00049 -0.00196 -0.00147 2.58705

R41 2.06269 -0.00012 -0.00011 -0.00004 -0.00016 2.06253

R42 2.07032 -0.00032 -0.00033 -0.00004 -0.00037 2.06995

R43 2.07032 -0.00032 -0.00033 -0.00004 -0.00037 2.06995

R44 2.06944 -0.00025 -0.00027 0.00033 0.00006 2.06950

R45 2.06944 -0.00025 -0.00027 0.00033 0.00006 2.06950

R46 2.06192 -0.00014 -0.00008 -0.00011 -0.00018 2.06173

R47 2.06944 -0.00025 -0.00027 0.00033 0.00006 2.06950

R48 2.06944 -0.00025 -0.00027 0.00033 0.00006 2.06950

R49 2.06192 -0.00014 -0.00008 -0.00011 -0.00018 2.06173

R50 2.07032 -0.00032 -0.00033 -0.00004 -0.00037 2.06995

R51 2.07032 -0.00032 -0.00033 -0.00004 -0.00037 2.06995

R52 2.06269 -0.00012 -0.00011 -0.00004 -0.00016 2.06253

A1 1.89235 0.00016 0.00020 0.00042 0.00062 1.89297

A2 2.20601 0.00001 -0.00084 -0.00008 -0.00092 2.20508

A3 2.18483 -0.00017 0.00064 -0.00033 0.00030 2.18513

A4 1.90637 -0.00007 0.00046 -0.00125 -0.00080 1.90557

A5 2.19026 0.00035 0.00286 -0.00044 0.00242 2.19268

A6 2.18655 -0.00028 -0.00331 0.00169 -0.00162 2.18493

A7 1.89565 -0.00005 -0.00054 0.00189 0.00135 1.89700

A8 2.21990 0.00056 0.00194 0.00125 0.00319 2.22309

A9 2.16763 -0.00050 -0.00140 -0.00313 -0.00454 2.16309

A10 1.85212 0.00005 -0.00026 -0.00140 -0.00166 1.85046

A11 2.17744 -0.00048 -0.00295 0.00102 -0.00193 2.17552

A12 2.25362 0.00043 0.00321 0.00037 0.00358 2.25721

A13 1.87828 -0.00008 0.00015 0.00034 0.00049 1.87877

A14 2.18239 -0.00009 -0.00151 0.00044 -0.00107 2.18132

A15 2.22251 0.00017 0.00136 -0.00078 0.00058 2.22309

A16 2.17214 -0.00084 0.00017 -0.00465 -0.00449 2.16765

A17 2.22847 0.00049 0.00065 0.00240 0.00305 2.23152

A18 2.16973 -0.00017 -0.00016 -0.00191 -0.00206 2.16766

A19 1.88499 -0.00032 -0.00049 -0.00049 -0.00098 1.88401

A20 1.91202 0.00034 0.00082 0.00150 0.00232 1.91433

A21 2.19044 -0.00019 -0.00210 0.00087 -0.00124 2.18920

A22 2.18072 -0.00015 0.00129 -0.00237 -0.00108 2.17965

A23 1.88638 -0.00035 -0.00045 -0.00193 -0.00238 1.88400

A24 2.24348 0.00080 0.00204 0.00227 0.00430 2.24778

A25 2.15333 -0.00045 -0.00159 -0.00034 -0.00193 2.15140

A26 1.85609 0.00015 -0.00026 0.00157 0.00131 1.85740

A27 2.15958 -0.00076 -0.00372 -0.00184 -0.00556 2.15403

A28 2.26751 0.00061 0.00398 0.00027 0.00425 2.27176

A29 1.88530 0.00018 0.00039 -0.00065 -0.00027 1.88504

A30 2.16730 -0.00028 -0.00184 -0.00057 -0.00241 2.16489

A31 2.23059 0.00010 0.00145 0.00122 0.00267 2.23326

A32 2.17318 -0.00075 -0.00269 -0.00093 -0.00362 2.16956

A33 1.85609 0.00015 -0.00026 0.00157 0.00131 1.85740

A34 2.26751 0.00061 0.00398 0.00027 0.00425 2.27176

A35 2.15958 -0.00076 -0.00372 -0.00184 -0.00556 2.15403

A36 1.88530 0.00018 0.00039 -0.00065 -0.00027 1.88504

A37 2.23059 0.00010 0.00145 0.00122 0.00267 2.23326

A38 2.16730 -0.00028 -0.00184 -0.00057 -0.00241 2.16489

A39 1.88499 -0.00032 -0.00049 -0.00049 -0.00098 1.88401

A40 2.16973 -0.00017 -0.00016 -0.00191 -0.00206 2.16766

A41 2.22847 0.00049 0.00065 0.00240 0.00305 2.23152

A42 1.91202 0.00034 0.00082 0.00150 0.00232 1.91433

A43 2.19044 -0.00019 -0.00210 0.00087 -0.00124 2.18920

A44 2.18072 -0.00015 0.00129 -0.00237 -0.00108 2.17965

A45 2.15333 -0.00045 -0.00159 -0.00034 -0.00193 2.15140

A46 2.24348 0.00080 0.00204 0.00227 0.00430 2.24778

A47 1.88638 -0.00035 -0.00045 -0.00193 -0.00238 1.88400

A48 2.17214 -0.00084 0.00017 -0.00465 -0.00449 2.16765

A49 1.90637 -0.00007 0.00046 -0.00125 -0.00080 1.90557

A50 2.18655 -0.00028 -0.00331 0.00169 -0.00162 2.18493

A51 2.19026 0.00035 0.00286 -0.00044 0.00242 2.19268

A52 2.21990 0.00056 0.00194 0.00125 0.00319 2.22309

A53 2.16763 -0.00050 -0.00140 -0.00313 -0.00454 2.16309

A54 1.89565 -0.00005 -0.00054 0.00189 0.00135 1.89700

A55 1.85212 0.00005 -0.00026 -0.00140 -0.00166 1.85046

A56 2.17744 -0.00048 -0.00295 0.00102 -0.00193 2.17552

A57 2.25362 0.00043 0.00321 0.00037 0.00358 2.25721

A58 1.87828 -0.00008 0.00015 0.00034 0.00049 1.87877

A59 2.22251 0.00017 0.00136 -0.00078 0.00058 2.22309

A60 2.18239 -0.00009 -0.00151 0.00044 -0.00107 2.18132

A61 1.89235 0.00016 0.00020 0.00042 0.00062 1.89297

A62 2.20601 0.00001 -0.00084 -0.00008 -0.00092 2.20508

A63 2.18483 -0.00017 0.00064 -0.00033 0.00030 2.18513

A64 2.17318 -0.00075 -0.00269 -0.00093 -0.00362 2.16956

A65 1.56887 0.00026 0.00266 -0.00155 0.00110 1.56998

A66 1.57272 -0.00026 -0.00266 0.00155 -0.00110 1.57162

A67 1.57272 -0.00026 -0.00266 0.00155 -0.00110 1.57162

A68 1.56887 0.00026 0.00266 -0.00155 0.00110 1.56998

A69 1.94082 0.00021 0.00174 0.00034 0.00207 1.94289

A70 1.94138 -0.00010 -0.00032 -0.00061 -0.00093 1.94045

A71 1.94138 -0.00010 -0.00032 -0.00061 -0.00093 1.94045

A72 1.88911 -0.00000 -0.00009 0.00083 0.00073 1.88984

A73 1.88911 -0.00000 -0.00009 0.00083 0.00073 1.88984

A74 1.85898 -0.00002 -0.00101 -0.00075 -0.00176 1.85722

A75 1.93393 -0.00000 -0.00038 0.00116 0.00078 1.93471

A76 1.93393 -0.00000 -0.00038 0.00116 0.00078 1.93471

A77 1.94352 0.00016 0.00202 -0.00078 0.00124 1.94476

A78 1.85947 -0.00011 -0.00124 -0.00143 -0.00267 1.85679

A79 1.89520 -0.00003 -0.00007 -0.00008 -0.00016 1.89504

A80 1.89520 -0.00003 -0.00007 -0.00008 -0.00016 1.89504

A81 1.93393 -0.00000 -0.00038 0.00116 0.00078 1.93471

A82 1.93393 -0.00000 -0.00038 0.00116 0.00078 1.93471

A83 1.94352 0.00016 0.00202 -0.00078 0.00124 1.94476

A84 1.85947 -0.00011 -0.00124 -0.00143 -0.00267 1.85679

A85 1.89520 -0.00003 -0.00007 -0.00008 -0.00016 1.89504

A86 1.89520 -0.00003 -0.00007 -0.00008 -0.00016 1.89504

A87 1.94138 -0.00010 -0.00032 -0.00061 -0.00093 1.94045

A88 1.94138 -0.00010 -0.00032 -0.00061 -0.00093 1.94045

A89 1.94082 0.00021 0.00174 0.00034 0.00207 1.94289

A90 1.85898 -0.00002 -0.00101 -0.00075 -0.00176 1.85722

A91 1.88911 -0.00000 -0.00009 0.00083 0.00073 1.88984

A92 1.88911 -0.00000 -0.00009 0.00083 0.00073 1.88984

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 1.03463 -0.00008 -0.00085 -0.00087 -0.00171 1.03292

D31 -1.03463 0.00008 0.00085 0.00087 0.00171 -1.03292

D32 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.10696 -0.00008 -0.00085 -0.00087 -0.00171 -2.10867

D34 2.10696 0.00008 0.00085 0.00087 0.00171 2.10867

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 1.03014 -0.00007 -0.00101 -0.00016 -0.00117 1.02897

D64 -1.03014 0.00007 0.00101 0.00016 0.00117 -1.02897

D65 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D66 -2.11145 -0.00007 -0.00101 -0.00016 -0.00117 -2.11262

D67 2.11145 0.00007 0.00101 0.00016 0.00117 2.11262

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 -2.11145 -0.00007 -0.00101 -0.00016 -0.00117 -2.11262

D80 2.11145 0.00007 0.00101 0.00016 0.00117 2.11262

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 1.03014 -0.00007 -0.00101 -0.00016 -0.00117 1.02897

D83 -1.03014 0.00007 0.00101 0.00016 0.00117 -1.02897

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 1.03463 -0.00008 -0.00085 -0.00087 -0.00171 1.03292

D126 -1.03463 0.00008 0.00085 0.00087 0.00171 -1.03292

D127 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D128 -2.10696 -0.00008 -0.00085 -0.00087 -0.00171 -2.10867

D129 2.10696 0.00008 0.00085 0.00087 0.00171 2.10867

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 0.001445 0.000450 NO

RMS Force 0.000327 0.000300 NO

Maximum Displacement 0.014747 0.001800 NO

RMS Displacement 0.003946 0.001200 NO

Predicted change in Energy=-5.003044D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:34:41 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 -2.071664 -2.191983 0.000000

2 7 0 -0.746120 -1.865588 0.000000

3 6 0 -0.006942 -3.003200 0.000000

4 6 0 -0.916421 -4.154988 0.000000

5 6 0 -2.188351 -3.634061 0.000000

6 7 0 1.353808 -3.106934 0.000000

7 6 0 2.177651 -2.073322 0.000000

8 7 0 1.856430 -0.744222 0.000000

9 6 0 2.996366 0.003728 0.000000

10 6 0 4.167999 -0.937772 0.000000

11 6 0 3.654494 -2.185890 0.000000

12 7 0 -3.123071 -1.315208 0.000000

13 6 0 -4.167999 0.937772 0.000000

14 6 0 -3.654494 2.185890 0.000000

15 6 0 -2.177651 2.073322 0.000000

16 7 0 -1.856430 0.744222 0.000000

17 6 0 -2.996366 -0.003728 0.000000

18 7 0 -1.353808 3.106934 0.000000

19 7 0 0.746120 1.865588 0.000000

20 6 0 0.006942 3.003200 0.000000

21 6 0 0.916421 4.154988 0.000000

22 6 0 2.188351 3.634061 0.000000

23 6 0 2.071664 2.191983 0.000000

24 7 0 3.123071 1.315208 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.479778 -5.578162 0.000000

27 1 0 -3.121321 -4.180435 0.000000

28 6 0 5.582581 -0.483634 0.000000

29 1 0 4.189920 -3.125342 0.000000

30 6 0 -5.582581 0.483634 0.000000

31 1 0 -4.189920 3.125342 0.000000

32 6 0 0.479778 5.578162 0.000000

33 1 0 3.121321 4.180435 0.000000

34 1 0 -1.335419 -6.255755 0.000000

35 1 0 0.136553 -5.803021 0.877162

36 1 0 0.136553 -5.803021 -0.877162

37 1 0 5.792395 0.138031 0.876830

38 1 0 5.792395 0.138031 -0.876830

39 1 0 6.272510 -1.328813 0.000000

40 1 0 -5.792395 -0.138031 0.876830

41 1 0 -5.792395 -0.138031 -0.876830

42 1 0 -6.272510 1.328813 0.000000

43 1 0 -0.136553 5.803021 0.877162

44 1 0 -0.136553 5.803021 -0.877162

45 1 0 1.335419 6.255755 0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.365138 0.000000

3 C 2.218367 1.356668 0.000000

4 C 2.277713 2.295726 1.467573 0.000000

5 C 1.446792 2.282001 2.270800 1.374471 0.000000

6 N 3.545560 2.439393 1.364698 2.500472 3.581167

7 C 4.250972 2.931142 2.374262 3.729158 4.636581

8 N 4.186399 2.833855 2.928334 4.395683 4.971059

9 C 5.523231 4.183365 4.249879 5.710063 6.333624

10 C 6.364468 5.000942 4.657910 6.016795 6.904576

11 C 5.726162 4.412256 3.751547 4.977008 6.019638

12 N 1.369010 2.439839 3.543950 3.596339 2.500156

13 C 3.766959 4.423582 5.731113 6.042264 4.982034

14 C 4.655225 4.987295 6.342814 6.906792 6.001784

15 C 4.266621 4.190977 5.521146 6.354726 5.707393

16 N 2.944082 2.836176 4.178968 4.988574 4.390846

17 C 2.375612 2.920638 4.234795 4.643181 3.719168

18 N 5.347320 5.009516 6.256819 7.275082 6.792457

19 N 4.940019 4.018513 4.926682 6.245909 6.233559

20 C 5.595581 4.926682 6.006416 7.217496 6.990890

21 C 7.015176 6.245909 7.217496 8.509701 8.385040

22 C 7.217376 6.233559 6.990890 8.385040 8.484169

23 C 6.032108 4.940019 5.595581 7.015176 7.217376

24 N 6.267828 5.008802 5.333444 6.800040 7.259922

25 Zn 3.016054 2.009257 3.003208 4.254850 4.242084

26 C 3.741700 3.722116 2.618016 1.488652 2.588195

27 H 2.248494 3.316640 3.329451 2.205047 1.081184

28 C 7.842572 6.477829 6.131148 7.464307 8.385260

29 H 6.330766 5.094259 4.198639 5.209116 6.398526

30 C 4.414234 5.376820 6.576152 6.579503 5.336311

31 H 5.723718 6.063756 7.419995 7.982418 7.049525

32 C 8.178326 7.544020 8.595154 9.832781 9.590828

33 H 8.220390 7.177151 7.835218 9.261892 9.447697

34 H 4.129928 4.429543 3.513399 2.142145 2.756950

35 H 4.322642 4.129396 2.937517 2.143404 3.298330

36 H 4.322642 4.129396 2.937517 2.143404 3.298330

37 H 8.248711 6.894600 6.653455 8.012931 8.870728

38 H 8.248711 6.894600 6.653455 8.012931 8.870728

39 H 8.388701 7.039126 6.498852 7.724506 8.769284

40 H 4.339514 5.405384 6.515328 6.378079 5.097077

41 H 4.339514 5.405384 6.515328 6.378079 5.097077

42 H 5.481159 6.383195 7.617328 7.665491 6.427323

43 H 8.272494 7.742645 8.850748 10.026941 9.697310

44 H 8.272494 7.742645 8.850748 10.026941 9.697310

45 H 9.108924 8.383855 9.355757 10.651496 10.498830

6 7 8 9 10

6 N 0.000000

7 C 1.321769 0.000000

8 N 2.415582 1.367366 0.000000

9 C 3.517700 2.232583 1.363408 0.000000

10 C 3.553159 2.291497 2.319658 1.503045 0.000000

11 C 2.478200 1.481126 2.304656 2.286386 1.349625

12 N 4.822108 5.354661 5.012131 6.259960 7.300833

13 C 6.844706 7.023814 6.254827 7.224996 8.544387

14 C 7.286774 7.221828 6.241461 6.999698 8.423103

15 C 6.269470 6.013594 4.920606 5.572583 7.023814

16 N 5.013684 4.920606 4.000100 4.908968 6.254827

17 C 5.343585 5.572583 4.908968 5.992737 7.224996

18 N 6.778151 6.269470 5.013684 5.343585 6.844706

19 N 5.009516 4.190977 2.836176 2.920638 4.423582

20 C 6.256819 5.521146 4.178968 4.234795 5.731113

21 C 7.275082 6.354726 4.988574 4.643181 6.042264

22 C 6.792457 5.707393 4.390846 3.719168 4.982034

23 C 5.347320 4.266621 2.944082 2.375612 3.766959

24 N 4.762943 3.517947 2.417773 1.317587 2.483504

25 Zn 3.389076 3.006797 2.000050 2.996368 4.272193

26 C 3.077175 4.398391 5.368878 6.575795 6.567729

27 H 4.602085 5.702547 6.048601 7.411702 7.978037

28 C 4.976367 3.757746 3.735252 2.631735 1.485693

29 H 2.836172 2.270676 3.333903 3.348977 2.187680

30 C 7.810613 8.170632 7.539663 8.592360 9.853640

31 H 8.341114 8.220223 7.178570 7.834997 9.293208

32 C 8.728965 7.837601 6.470526 6.116170 7.487348

33 H 7.498657 6.324555 5.084506 4.178577 5.224134

34 H 4.140896 5.462089 6.369059 7.612194 7.653011

35 H 3.085452 4.341216 5.414688 6.531943 6.379078

36 H 3.085452 4.341216 5.414688 6.531943 6.379078

37 H 5.567736 4.327272 4.127835 2.933368 2.136549

38 H 5.567736 4.327272 4.127835 2.933368 2.136549

39 H 5.230233 4.161990 4.454605 3.536776 2.140532

40 H 7.787903 8.248383 7.722748 8.833530 10.030846

41 H 7.787903 8.248383 7.722748 8.833530 10.030846

42 H 8.822504 9.109322 8.389109 9.363114 10.683709

43 H 9.076226 8.256012 6.899839 6.649541 8.045923

44 H 9.076226 8.256012 6.899839 6.649541 8.045923

45 H 9.362707 8.371552 7.019340 6.468895 7.731128

11 12 13 14 15

11 C 0.000000

12 N 6.833262 0.000000

13 C 8.423103 2.483504 0.000000

14 C 8.516676 3.541200 1.349625 0.000000

15 C 7.221828 3.517947 2.291497 1.481126 0.000000

16 N 6.241461 2.417773 2.319658 2.304656 1.367366

17 C 6.999698 1.317587 1.503045 2.286386 2.232583

18 N 7.286774 4.762943 3.553159 2.478200 1.321769

19 N 4.987295 5.008802 5.000942 4.412256 2.931142

20 C 6.342814 5.333444 4.657910 3.751547 2.374262

21 C 6.906792 6.800040 6.016795 4.977008 3.729158

22 C 6.001784 7.259922 6.904576 6.019638 4.636581

23 C 4.655225 6.267828 6.364468 5.726162 4.250972

24 N 3.541200 6.777417 7.300833 6.833262 5.354661

25 Zn 4.258338 3.388708 4.272193 4.258338 3.006797

26 C 5.347870 5.015953 7.487348 8.388047 7.837601

27 H 7.063277 2.865228 5.224134 6.388613 6.324555

28 C 2.572003 8.745279 9.853640 9.615088 8.170632

29 H 1.081319 7.533686 9.293208 9.473332 8.220223

30 C 9.615088 3.047134 1.485693 2.572003 3.757746

31 H 9.473332 4.566908 2.187680 1.081319 2.270676

32 C 8.388047 7.778115 6.567729 5.347870 4.398391

33 H 6.388613 8.318325 7.978037 7.063277 5.702547

34 H 6.439180 5.254018 7.731128 8.754398 8.371552

35 H 5.121422 5.615606 8.045923 8.886178 8.256012

36 H 5.121422 5.615606 8.045923 8.886178 8.256012

37 H 3.277204 9.075587 10.030846 9.705992 8.248383

38 H 3.277204 9.075587 10.030846 9.705992 8.248383

39 H 2.754739 9.395591 10.683709 10.530838 9.109322

40 H 9.705992 3.046288 2.136549 3.277204 4.327272

41 H 9.705992 3.046288 2.136549 3.277204 4.327272

42 H 10.530838 4.112154 2.140532 2.754739 4.161990

43 H 8.886178 7.769034 6.379078 5.121422 4.341216

44 H 8.886178 7.769034 6.379078 5.121422 4.341216

45 H 8.754398 8.786218 7.653011 6.439180 5.462089

16 17 18 19 20

16 N 0.000000

17 C 1.363408 0.000000

18 N 2.415582 3.517700 0.000000

19 N 2.833855 4.183365 2.439393 0.000000

20 C 2.928334 4.249879 1.364698 1.356668 0.000000

21 C 4.395683 5.710063 2.500472 2.295726 1.467573

22 C 4.971059 6.333624 3.581167 2.282001 2.270800

23 C 4.186399 5.523231 3.545560 1.365138 2.218367

24 N 5.012131 6.259960 4.822108 2.439839 3.543950

25 Zn 2.000050 2.996368 3.389076 2.009257 3.003208

26 C 6.470526 6.116170 8.728965 7.544020 8.595154

27 H 5.084506 4.178577 7.498657 7.177151 7.835218

28 C 7.539663 8.592360 7.810613 5.376820 6.576152

29 H 7.178570 7.834997 8.341114 6.063756 7.419995

30 C 3.735252 2.631735 4.976367 6.477829 6.131148

31 H 3.333903 3.348977 2.836172 5.094259 4.198639

32 C 5.368878 6.575795 3.077175 3.722116 2.618016

33 H 6.048601 7.411702 4.602085 3.316640 3.329451

34 H 7.019340 6.468895 9.362707 8.383855 9.355757

35 H 6.899839 6.649541 9.076226 7.742645 8.850748

36 H 6.899839 6.649541 9.076226 7.742645 8.850748

37 H 7.722748 8.833530 7.787903 5.405384 6.515328

38 H 7.722748 8.833530 7.787903 5.405384 6.515328

39 H 8.389109 9.363114 8.822504 6.383195 7.617328

40 H 4.127835 2.933368 5.567736 6.894600 6.653455

41 H 4.127835 2.933368 5.567736 6.894600 6.653455

42 H 4.454605 3.536776 5.230233 7.039126 6.498852

43 H 5.414688 6.531943 3.085452 4.129396 2.937517

44 H 5.414688 6.531943 3.085452 4.129396 2.937517

45 H 6.369059 7.612194 4.140896 4.429543 3.513399

21 22 23 24 25

21 C 0.000000

22 C 1.374471 0.000000

23 C 2.277713 1.446792 0.000000

24 N 3.596339 2.500156 1.369010 0.000000

25 Zn 4.254850 4.242084 3.016054 3.388708 0.000000

26 C 9.832781 9.590828 8.178326 7.778115 5.598757

27 H 9.261892 9.447697 8.220390 8.318325 5.217153

28 C 6.579503 5.336311 4.414234 3.047134 5.603492

29 H 7.982418 7.049525 5.723718 4.566908 5.227159

30 C 7.464307 8.385260 7.842572 8.745279 5.603492

31 H 5.209116 6.398526 6.330766 7.533686 5.227159

32 C 1.488652 2.588195 3.741700 5.015953 5.598757

33 H 2.205047 1.081184 2.248494 2.865228 5.217153

34 H 10.651496 10.498830 9.108924 8.786218 6.396704

35 H 10.026941 9.697310 8.272494 7.769034 5.870529

36 H 10.026941 9.697310 8.272494 7.769034 5.870529

37 H 6.378079 5.097077 4.339514 3.046288 5.860011

38 H 6.378079 5.097077 4.339514 3.046288 5.860011

39 H 7.665491 6.427323 5.481159 4.112154 6.411718

40 H 8.012931 8.870728 8.248711 9.075587 5.860011

41 H 8.012931 8.870728 8.248711 9.075587 5.860011

42 H 7.724506 8.769284 8.388701 9.395591 6.411718

43 H 2.143404 3.298330 4.322642 5.615606 5.870529

44 H 2.143404 3.298330 4.322642 5.615606 5.870529

45 H 2.142145 2.756950 4.129928 5.254018 6.396704

26 27 28 29 30

26 C 0.000000

27 H 2.988543 0.000000

28 C 7.918739 9.456440 0.000000

29 H 5.274695 7.386980 2.986323 0.000000

30 C 7.923634 5.273646 11.206983 10.417605 0.000000

31 H 9.461297 7.383514 10.417605 10.454318 2.986323

32 C 11.197515 10.401834 7.923634 9.461297 7.918739

33 H 10.401834 10.434306 5.273646 7.383514 9.456440

34 H 1.091446 2.737955 9.009779 6.350501 7.966038

35 H 1.095371 3.743787 7.663193 4.936514 8.544000

36 H 1.095371 3.743787 7.663193 4.936514 8.544000

37 H 8.531345 9.943456 1.095135 3.739834 11.413955

38 H 8.531345 9.943456 1.095135 3.739834 11.413955

39 H 7.978117 9.817118 1.091022 2.750399 11.992838

40 H 7.654264 4.923871 11.413955 10.456552 1.095135

41 H 7.654264 4.923871 11.413955 10.456552 1.095135

42 H 9.014547 6.346795 11.992838 11.371101 1.091022

43 H 11.420095 10.456943 8.544000 9.960093 7.663193

44 H 11.420095 10.456943 8.544000 9.960093 7.663193

45 H 11.972324 11.347979 7.966038 9.805772 9.009779

31 32 33 34 35

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32 C 5.274695 0.000000

33 H 7.386980 2.988543 0.000000

34 H 9.805772 11.972324 11.347979 0.000000

35 H 9.960093 11.420095 10.456943 1.772310 0.000000

36 H 9.960093 11.420095 10.456943 1.772310 1.754324

37 H 10.456552 7.654264 4.923871 9.615356 8.202723

38 H 10.456552 7.654264 4.923871 9.615356 8.388155

39 H 11.371101 9.014547 6.346795 9.063958 7.644470

40 H 3.739834 8.531345 9.943456 7.619712 8.200277

41 H 3.739834 8.531345 9.943456 7.619712 8.385763

42 H 2.750399 7.978117 9.817118 9.049892 9.628529

43 H 4.936514 1.095371 3.743787 12.149930 11.609255

44 H 4.936514 1.095371 3.743787 12.149930 11.741059

45 H 6.350501 1.091446 2.737955 12.793408 12.149930

36 37 38 39 40

36 H 0.000000

37 H 8.388155 0.000000

38 H 8.202723 1.753660 0.000000

39 H 7.644470 1.775098 1.775098 0.000000

40 H 8.385763 11.588079 11.720021 12.155193 0.000000

41 H 8.200277 11.720021 11.588079 12.155193 1.753660

42 H 9.628529 12.155193 12.155193 12.823435 1.775098

43 H 11.741059 8.200277 8.385763 9.628529 8.202723

44 H 11.609255 8.385763 8.200277 9.628529 8.388155

45 H 12.149930 7.619712 7.619712 9.049892 9.615356

41 42 43 44 45

41 H 0.000000

42 H 1.775098 0.000000

43 H 8.388155 7.644470 0.000000

44 H 8.202723 7.644470 1.754324 0.000000

45 H 9.615356 9.063958 1.772310 1.772310 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=0 Diff= 1.11D-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

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1 6 0 2.944580 -0.652708 0.000000

2 7 0 1.984041 0.317325 0.000000

3 6 0 2.580901 1.535646 0.000000

4 6 0 4.036217 1.346368 0.000000

5 6 0 4.242066 -0.012600 0.000000

6 7 0 1.971425 2.756686 0.000000

7 6 0 0.661487 2.933132 0.000000

8 7 0 -0.314254 1.975207 0.000000

9 6 0 -1.541294 2.569560 0.000000

10 6 0 -1.334725 4.058343 0.000000

11 6 0 0.000000 4.258338 0.000000

12 7 0 2.731843 -2.005088 0.000000

13 6 0 1.334725 -4.058343 0.000000

14 6 0 -0.000000 -4.258338 0.000000

15 6 0 -0.661487 -2.933132 0.000000

16 7 0 0.314254 -1.975207 0.000000

17 6 0 1.541294 -2.569560 0.000000

18 7 0 -1.971425 -2.756686 0.000000

19 7 0 -1.984041 -0.317325 0.000000

20 6 0 -2.580901 -1.535646 0.000000

21 6 0 -4.036217 -1.346368 0.000000

22 6 0 -4.242066 0.012600 0.000000

23 6 0 -2.944580 0.652708 0.000000

24 7 0 -2.731843 2.005088 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 5.033443 2.451639 0.000000

27 1 0 5.189875 -0.532808 0.000000

28 6 0 -2.450598 5.039215 0.000000

29 1 0 0.531390 5.200079 0.000000

30 6 0 2.450598 -5.039215 0.000000

31 1 0 -0.531390 -5.200079 0.000000

32 6 0 -5.033443 -2.451639 0.000000

33 1 0 -5.189875 0.532808 0.000000

34 1 0 6.054170 2.065152 0.000000

35 1 0 4.910042 3.095996 0.877162

36 1 0 4.910042 3.095996 -0.877162

37 1 0 -3.091810 4.900164 0.876830

38 1 0 -3.091810 4.900164 -0.876830

39 1 0 -2.079421 6.065157 0.000000

40 1 0 3.091810 -4.900164 0.876830

41 1 0 3.091810 -4.900164 -0.876830

42 1 0 2.079421 -6.065157 0.000000

43 1 0 -4.910042 -3.095996 0.877162

44 1 0 -4.910042 -3.095996 -0.877162

45 1 0 -6.054170 -2.065152 0.000000

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

Rotational constants (GHZ): 0.1828866 0.1820130 0.0914291

Leave Link 202 at Tue Sep 17 14:34:41 2019, MaxMem= 2415919104 cpu: 0.1

(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 101 beta electrons

nuclear repulsion energy 2761.8556421520 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= -0.1142082474 Hartrees.

Nuclear repulsion after empirical dispersion term = 2761.7414339046 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 = 3594

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.36D-07

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 248

GePol: Fraction of low-weight points (<1% of avg) = 6.90%

GePol: Cavity surface area = 378.520 Ang\*\*2

GePol: Cavity volume = 378.206 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0107046459 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2761.7307292588 Hartrees.

Leave Link 301 at Tue Sep 17 14:34:41 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= 15327 LenP2D= 41274.

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 14:34:42 2019, MaxMem= 2415919104 cpu: 12.3

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:34:42 2019, MaxMem= 2415919104 cpu: 1.2

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= -0.000000 -0.000000 0.000000

Rot= 1.000000 -0.000000 -0.000000 -0.000225 Ang= -0.03 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 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0177 S= 1.0059

Leave Link 401 at Tue Sep 17 14:34:43 2019, MaxMem= 2415919104 cpu: 22.8

(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= 38750508.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.66D-15 for 3588.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.33D-15 for 3337 2097.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.77D-15 for 3588.

Iteration 1 A^-1\*A deviation from orthogonality is 7.22D-12 for 1745 1741.

E= -1275.84268885374

DIIS: error= 2.52D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.84268885374 IErMin= 1 ErrMin= 2.52D-04

ErrMax= 2.52D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.85D-04 BMatP= 1.85D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 2.52D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.303 Goal= None Shift= 0.000

Gap= 0.393 Goal= None Shift= 0.000

RMSDP=2.12D-05 MaxDP=5.24D-04 OVMax= 1.81D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.11D-05 CP: 1.00D+00

E= -1275.84275008830 Delta-E= -0.000061234557 Rises=F Damp=F

DIIS: error= 8.02D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84275008830 IErMin= 2 ErrMin= 8.02D-05

ErrMax= 8.02D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.29D-05 BMatP= 1.85D-04

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

Coeff-Com: 0.581D-01 0.942D+00

Coeff: 0.581D-01 0.942D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=5.55D-06 MaxDP=3.31D-04 DE=-6.12D-05 OVMax= 1.60D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 5.53D-06 CP: 1.00D+00 1.02D+00

E= -1275.84274722003 Delta-E= 0.000002868270 Rises=F Damp=F

DIIS: error= 1.29D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1275.84275008830 IErMin= 2 ErrMin= 8.02D-05

ErrMax= 1.29D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.95D-05 BMatP= 1.29D-05

IDIUse=3 WtCom= 4.68D-01 WtEn= 5.32D-01

Coeff-Com: -0.279D-01 0.619D+00 0.408D+00

Coeff-En: 0.000D+00 0.647D+00 0.353D+00

Coeff: -0.131D-01 0.634D+00 0.379D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.42D-06 MaxDP=1.71D-04 DE= 2.87D-06 OVMax= 4.88D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.68D-06 CP: 1.00D+00 1.04D+00 4.71D-01

E= -1275.84275320158 Delta-E= -0.000005981548 Rises=F Damp=F

DIIS: error= 1.78D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84275320158 IErMin= 4 ErrMin= 1.78D-05

ErrMax= 1.78D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.32D-07 BMatP= 1.29D-05

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

Coeff-Com: -0.144D-01 0.237D+00 0.151D+00 0.626D+00

Coeff: -0.144D-01 0.237D+00 0.151D+00 0.626D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=8.86D-07 MaxDP=4.21D-05 DE=-5.98D-06 OVMax= 4.89D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 8.11D-07 CP: 1.00D+00 1.05D+00 5.30D-01 1.02D+00

E= -1275.84275331345 Delta-E= -0.000000111873 Rises=F Damp=F

DIIS: error= 1.58D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84275331345 IErMin= 5 ErrMin= 1.58D-05

ErrMax= 1.58D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.36D-07 BMatP= 3.32D-07

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

Coeff-Com: -0.376D-02 0.363D-01 0.172D-01 0.377D+00 0.573D+00

Coeff: -0.376D-02 0.363D-01 0.172D-01 0.377D+00 0.573D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=5.47D-07 MaxDP=2.05D-05 DE=-1.12D-07 OVMax= 3.26D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.41D-07 CP: 1.00D+00 1.05D+00 5.48D-01 1.25D+00 1.19D+00

E= -1275.84275338198 Delta-E= -0.000000068523 Rises=F Damp=F

DIIS: error= 9.91D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84275338198 IErMin= 6 ErrMin= 9.91D-06

ErrMax= 9.91D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.20D-08 BMatP= 1.36D-07

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

Coeff-Com: 0.865D-03-0.242D-01-0.224D-01 0.740D-01 0.198D+00 0.774D+00

Coeff: 0.865D-03-0.242D-01-0.224D-01 0.740D-01 0.198D+00 0.774D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=5.84D-07 MaxDP=2.99D-05 DE=-6.85D-08 OVMax= 4.34D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.26D-07 CP: 1.00D+00 1.05D+00 5.83D-01 1.43D+00 1.63D+00

CP: 1.45D+00

E= -1275.84275342370 Delta-E= -0.000000041721 Rises=F Damp=F

DIIS: error= 8.31D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84275342370 IErMin= 7 ErrMin= 8.31D-06

ErrMax= 8.31D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.99D-08 BMatP= 2.20D-08

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

Coeff-Com: 0.266D-02-0.350D-01-0.282D-01-0.132D+00-0.222D+00 0.584D+00

Coeff-Com: 0.830D+00

Coeff: 0.266D-02-0.350D-01-0.282D-01-0.132D+00-0.222D+00 0.584D+00

Coeff: 0.830D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=7.16D-07 MaxDP=3.43D-05 DE=-4.17D-08 OVMax= 5.28D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.27D-07 CP: 1.00D+00 1.05D+00 6.21D-01 1.67D+00 2.14D+00

CP: 2.39D+00 1.57D+00

E= -1275.84275346569 Delta-E= -0.000000041992 Rises=F Damp=F

DIIS: error= 5.83D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84275346569 IErMin= 8 ErrMin= 5.83D-06

ErrMax= 5.83D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.41D-09 BMatP= 1.99D-08

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

Coeff-Com: 0.650D-03 0.965D-04-0.255D-02-0.914D-01-0.276D+00-0.131D+00

Coeff-Com: 0.219D+00 0.128D+01

Coeff: 0.650D-03 0.965D-04-0.255D-02-0.914D-01-0.276D+00-0.131D+00

Coeff: 0.219D+00 0.128D+01

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=9.34D-07 MaxDP=4.92D-05 DE=-4.20D-08 OVMax= 7.15D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.10D-07 CP: 1.00D+00 1.06D+00 6.71D-01 1.96D+00 2.82D+00

CP: 3.00D+00 2.77D+00 2.01D+00

E= -1275.84275349680 Delta-E= -0.000000031111 Rises=F Damp=F

DIIS: error= 3.48D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84275349680 IErMin= 9 ErrMin= 3.48D-06

ErrMax= 3.48D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.75D-09 BMatP= 6.41D-09

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

Coeff-Com: -0.641D-03 0.146D-01 0.831D-02 0.114D-02-0.102D+00-0.285D+00

Coeff-Com: -0.266D+00 0.940D+00 0.689D+00

Coeff: -0.641D-03 0.146D-01 0.831D-02 0.114D-02-0.102D+00-0.285D+00

Coeff: -0.266D+00 0.940D+00 0.689D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.73D-07 MaxDP=2.39D-05 DE=-3.11D-08 OVMax= 3.60D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.77D-07 CP: 1.00D+00 1.06D+00 6.94D-01 2.10D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.79D+00 1.96D+00

E= -1275.84275350542 Delta-E= -0.000000008619 Rises=F Damp=F

DIIS: error= 1.60D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84275350542 IErMin=10 ErrMin= 1.60D-06

ErrMax= 1.60D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.84D-10 BMatP= 4.75D-09

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

Coeff-Com: -0.542D-03 0.703D-02 0.387D-02 0.393D-01 0.467D-01-0.569D-01

Coeff-Com: -0.246D+00 0.158D-01 0.258D+00 0.933D+00

Coeff: -0.542D-03 0.703D-02 0.387D-02 0.393D-01 0.467D-01-0.569D-01

Coeff: -0.246D+00 0.158D-01 0.258D+00 0.933D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.52D-07 MaxDP=1.34D-05 DE=-8.62D-09 OVMax= 1.95D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 8.98D-08 CP: 1.00D+00 1.06D+00 7.07D-01 2.17D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.52D+00 1.82D+00

E= -1275.84275350787 Delta-E= -0.000000002451 Rises=F Damp=F

DIIS: error= 7.72D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84275350787 IErMin=11 ErrMin= 7.72D-07

ErrMax= 7.72D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.08D-10 BMatP= 8.84D-10

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

Coeff-Com: -0.255D-04-0.243D-02-0.214D-02 0.226D-01 0.630D-01 0.112D+00

Coeff-Com: -0.354D-01-0.378D+00-0.205D+00 0.486D+00 0.939D+00

Coeff: -0.255D-04-0.243D-02-0.214D-02 0.226D-01 0.630D-01 0.112D+00

Coeff: -0.354D-01-0.378D+00-0.205D+00 0.486D+00 0.939D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.60D-07 MaxDP=8.56D-06 DE=-2.45D-09 OVMax= 1.22D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 3.69D-08 CP: 1.00D+00 1.06D+00 7.14D-01 2.20D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.89D+00 2.36D+00

CP: 1.66D+00

E= -1275.84275350867 Delta-E= -0.000000000802 Rises=F Damp=F

DIIS: error= 3.65D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84275350867 IErMin=12 ErrMin= 3.65D-07

ErrMax= 3.65D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.13D-10 BMatP= 4.08D-10

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

Coeff-Com: 0.101D-03-0.301D-02-0.235D-02 0.528D-02 0.235D-01 0.785D-01

Coeff-Com: 0.200D-01-0.206D+00-0.170D+00 0.101D+00 0.528D+00 0.626D+00

Coeff: 0.101D-03-0.301D-02-0.235D-02 0.528D-02 0.235D-01 0.785D-01

Coeff: 0.200D-01-0.206D+00-0.170D+00 0.101D+00 0.528D+00 0.626D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.63D-08 MaxDP=2.43D-06 DE=-8.02D-10 OVMax= 3.49D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.11D-08 CP: 1.00D+00 1.06D+00 7.16D-01 2.22D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.99D+00 2.51D+00

CP: 1.85D+00 1.17D+00

E= -1275.84275350880 Delta-E= -0.000000000129 Rises=F Damp=F

DIIS: error= 1.93D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84275350880 IErMin=13 ErrMin= 1.93D-07

ErrMax= 1.93D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.26D-11 BMatP= 1.13D-10

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

Coeff-Com: 0.542D-04-0.498D-03-0.457D-03-0.504D-02-0.131D-01-0.140D-02

Coeff-Com: 0.149D-01 0.453D-01-0.102D-01-0.131D+00-0.980D-01 0.343D+00

Coeff-Com: 0.856D+00

Coeff: 0.542D-04-0.498D-03-0.457D-03-0.504D-02-0.131D-01-0.140D-02

Coeff: 0.149D-01 0.453D-01-0.102D-01-0.131D+00-0.980D-01 0.343D+00

Coeff: 0.856D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.32D-08 MaxDP=1.74D-06 DE=-1.29D-10 OVMax= 2.49D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 1.53D-08 CP: 1.00D+00 1.06D+00 7.17D-01 2.23D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 3.00D+00 2.61D+00

CP: 1.97D+00 1.35D+00 1.26D+00

E= -1275.84275350884 Delta-E= -0.000000000037 Rises=F Damp=F

DIIS: error= 1.04D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84275350884 IErMin=14 ErrMin= 1.04D-07

ErrMax= 1.04D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.55D-12 BMatP= 3.26D-11

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

Coeff-Com: 0.614D-06 0.619D-03 0.416D-03-0.388D-02-0.132D-01-0.230D-01

Coeff-Com: -0.294D-03 0.831D-01 0.443D-01-0.950D-01-0.212D+00-0.894D-03

Coeff-Com: 0.425D+00 0.795D+00

Coeff: 0.614D-06 0.619D-03 0.416D-03-0.388D-02-0.132D-01-0.230D-01

Coeff: -0.294D-03 0.831D-01 0.443D-01-0.950D-01-0.212D+00-0.894D-03

Coeff: 0.425D+00 0.795D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.57D-08 MaxDP=7.68D-07 DE=-3.73D-11 OVMax= 1.14D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 2.92D-09 CP: 1.00D+00 1.06D+00 7.18D-01 2.23D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 3.00D+00 2.66D+00

CP: 2.03D+00 1.41D+00 1.58D+00 1.48D+00

E= -1275.84275350886 Delta-E= -0.000000000026 Rises=F Damp=F

DIIS: error= 5.80D-08 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.84275350886 IErMin=15 ErrMin= 5.80D-08

ErrMax= 5.80D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.71D-12 BMatP= 7.55D-12

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

Coeff-Com: -0.161D-04 0.472D-03 0.354D-03-0.461D-03-0.271D-02-0.116D-01

Coeff-Com: -0.523D-02 0.287D-01 0.261D-01-0.659D-02-0.775D-01-0.968D-01

Coeff-Com: -0.504D-01 0.375D+00 0.821D+00

Coeff: -0.161D-04 0.472D-03 0.354D-03-0.461D-03-0.271D-02-0.116D-01

Coeff: -0.523D-02 0.287D-01 0.261D-01-0.659D-02-0.775D-01-0.968D-01

Coeff: -0.504D-01 0.375D+00 0.821D+00

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=6.08D-09 MaxDP=2.76D-07 DE=-2.59D-11 OVMax= 3.91D-06

Error on total polarization charges = 0.06476

SCF Done: E(UB3LYP) = -1275.84275351 A.U. after 15 cycles

NFock= 15 Conv=0.61D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0178 S= 1.0059

<L.S>= 0.000000000000E+00

KE= 1.320803102858D+03 PE=-8.575411717768D+03 EE= 3.217035132142D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.72

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0178, after 2.0002

Leave Link 502 at Tue Sep 17 14:36:01 2019, MaxMem= 2415919104 cpu: 1365.1

(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= 15327 LenP2D= 41274.

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 14:36:05 2019, MaxMem= 2415919104 cpu: 72.2

(Enter /home/blab/g09/l702.exe)

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

Leave Link 702 at Tue Sep 17 14:36:05 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 14:36:15 2019, MaxMem= 2415919104 cpu: 177.3

(Enter /home/blab/g09/l716.exe)

Dipole =-3.81916720D-13 6.39488462D-14 4.44089210D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000638806 -0.000264461 0.000000000

2 7 0.000348044 0.000409784 0.000000000

3 6 0.000368422 -0.000336429 -0.000000000

4 6 -0.000179141 0.000641937 -0.000000000

5 6 -0.000279316 0.000129010 -0.000000000

6 7 0.000533704 0.000652399 0.000000000

7 6 -0.000274802 -0.000568886 0.000000000

8 7 -0.001434295 0.000459137 0.000000000

9 6 0.000305988 0.000642401 0.000000000

10 6 0.000630751 0.000127460 0.000000000

11 6 0.000144600 0.000225361 0.000000000

12 7 0.000247892 0.000857374 0.000000000

13 6 -0.000630751 -0.000127460 0.000000000

14 6 -0.000144600 -0.000225361 -0.000000000

15 6 0.000274802 0.000568886 0.000000000

16 7 0.001434295 -0.000459137 -0.000000000

17 6 -0.000305988 -0.000642401 0.000000000

18 7 -0.000533704 -0.000652399 -0.000000000

19 7 -0.000348044 -0.000409784 0.000000000

20 6 -0.000368422 0.000336429 -0.000000000

21 6 0.000179141 -0.000641937 0.000000000

22 6 0.000279316 -0.000129010 -0.000000000

23 6 0.000638806 0.000264461 0.000000000

24 7 -0.000247892 -0.000857374 -0.000000000

25 30 0.000000000 -0.000000000 -0.000000000

26 6 0.000291435 -0.000037026 -0.000000000

27 1 -0.000018780 0.000132915 0.000000000

28 6 0.000175508 0.000119415 -0.000000000

29 1 -0.000054396 0.000115049 -0.000000000

30 6 -0.000175508 -0.000119415 -0.000000000

31 1 0.000054396 -0.000115049 0.000000000

32 6 -0.000291435 0.000037026 0.000000000

33 1 0.000018780 -0.000132915 0.000000000

34 1 0.000092728 0.000011985 0.000000000

35 1 -0.000126416 0.000010083 -0.000111470

36 1 -0.000126416 0.000010083 0.000111470

37 1 -0.000162179 -0.000195759 -0.000150915

38 1 -0.000162179 -0.000195759 0.000150915

39 1 0.000025861 0.000079714 -0.000000000

40 1 0.000162179 0.000195759 -0.000150915

41 1 0.000162179 0.000195759 0.000150915

42 1 -0.000025861 -0.000079714 0.000000000

43 1 0.000126416 -0.000010083 -0.000111470

44 1 0.000126416 -0.000010083 0.000111470

45 1 -0.000092728 -0.000011985 -0.000000000

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

Cartesian Forces: Max 0.001434295 RMS 0.000325104

Leave Link 716 at Tue Sep 17 14:36:15 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 0.001032165 RMS 0.000186162

Search for a local minimum.

Step number 27 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 12 13 14 15

16 17 18 19 20

21 22 23 24 25

26 27

DE= -5.24D-05 DEPred=-5.00D-05 R= 1.05D+00

TightC=F SS= 1.41D+00 RLast= 2.55D-02 DXNew= 8.4090D-02 7.6585D-02

Trust test= 1.05D+00 RLast= 2.55D-02 DXMaxT set to 7.66D-02

ITU= 1 -1 1 -1 -1 1 0 0 1 -1 -1 1 1 -1 1 1 1 -1 0 1

ITU= -1 1 1 1 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01336

Eigenvalues --- 0.01337 0.01346 0.01347 0.01604 0.01623

Eigenvalues --- 0.01631 0.01639 0.01693 0.01774 0.01793

Eigenvalues --- 0.01809 0.01823 0.01890 0.01910 0.01939

Eigenvalues --- 0.01950 0.01997 0.02000 0.02045 0.02047

Eigenvalues --- 0.02070 0.02087 0.02103 0.02110 0.02115

Eigenvalues --- 0.02205 0.02312 0.02316 0.02351 0.02372

Eigenvalues --- 0.06103 0.07095 0.07196 0.07196 0.07197

Eigenvalues --- 0.07197 0.07315 0.07384 0.07504 0.12378

Eigenvalues --- 0.14328 0.14498 0.14500 0.15405 0.15980

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16091 0.16212 0.16544 0.17739 0.19339

Eigenvalues --- 0.20563 0.22059 0.22090 0.23404 0.23842

Eigenvalues --- 0.23854 0.24062 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25193 0.25234

Eigenvalues --- 0.25816 0.27917 0.29018 0.30702 0.32569

Eigenvalues --- 0.33187 0.33197 0.33282 0.33282 0.33309

Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33732 0.33787 0.34395 0.34437

Eigenvalues --- 0.34437 0.34455 0.34973 0.35555 0.35564

Eigenvalues --- 0.35643 0.35682 0.35682 0.35744 0.37371

Eigenvalues --- 0.38075 0.41641 0.41812 0.42936 0.45666

Eigenvalues --- 0.46801 0.48967 0.48977 0.51201 0.51358

Eigenvalues --- 0.51361 0.52428 0.53339 0.54020 0.54028

Eigenvalues --- 0.55536 0.56319 0.56327 0.96795

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 1.03246 -0.09574 0.05694 -0.00757 0.01392

Cosine: 0.896 > 0.670

Length: 0.756

GDIIS step was calculated using 5 of the last 27 vectors.

Iteration 1 RMS(Cart)= 0.00072828 RMS(Int)= 0.00000058

Iteration 2 RMS(Cart)= 0.00000038 RMS(Int)= 0.00000055

ITry= 1 IFail=0 DXMaxC= 2.93D-03 DCOld= 1.00D+10 DXMaxT= 7.66D-02 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 4.13D-10 for atom 43.

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

(Linear) (Quad) (Total)

R1 2.57974 0.00043 0.00098 0.00014 0.00112 2.58086

R2 2.73404 -0.00046 -0.00091 -0.00038 -0.00129 2.73275

R3 2.58705 -0.00025 -0.00004 0.00019 0.00016 2.58721

R4 2.56373 -0.00004 -0.00066 0.00080 0.00015 2.56388

R5 3.79694 -0.00065 0.00024 -0.00247 -0.00223 3.79471

R6 2.77331 -0.00013 -0.00046 -0.00097 -0.00142 2.77189

R7 2.57890 0.00022 0.00049 -0.00003 0.00046 2.57937

R8 2.59737 0.00020 0.00053 0.00016 0.00069 2.59806

R9 2.81314 0.00004 -0.00002 0.00017 0.00015 2.81329

R10 2.04314 -0.00005 -0.00001 -0.00013 -0.00014 2.04300

R11 2.49778 -0.00062 0.00018 -0.00052 -0.00034 2.49744

R12 2.58395 0.00003 -0.00072 0.00080 0.00008 2.58402

R13 2.79892 0.00027 0.00019 -0.00020 -0.00001 2.79891

R14 2.57647 0.00037 0.00103 0.00014 0.00118 2.57764

R15 3.77955 -0.00064 0.00018 -0.00298 -0.00280 3.77674

R16 2.84034 0.00012 -0.00077 -0.00014 -0.00092 2.83943

R17 2.48988 -0.00103 -0.00057 0.00003 -0.00054 2.48934

R18 2.55042 -0.00018 0.00006 -0.00014 -0.00008 2.55034

R19 2.80755 -0.00017 0.00010 -0.00011 -0.00001 2.80755

R20 2.04340 -0.00013 -0.00003 -0.00008 -0.00011 2.04329

R21 2.48988 -0.00103 -0.00057 0.00003 -0.00054 2.48934

R22 2.55042 -0.00018 0.00006 -0.00014 -0.00008 2.55034

R23 2.84034 0.00012 -0.00077 -0.00014 -0.00092 2.83943

R24 2.80755 -0.00017 0.00010 -0.00011 -0.00001 2.80755

R25 2.79892 0.00027 0.00019 -0.00020 -0.00001 2.79891

R26 2.04340 -0.00013 -0.00003 -0.00008 -0.00011 2.04329

R27 2.58395 0.00003 -0.00072 0.00080 0.00008 2.58402

R28 2.49778 -0.00062 0.00018 -0.00052 -0.00034 2.49744

R29 2.57647 0.00037 0.00103 0.00014 0.00118 2.57764

R30 3.77955 -0.00064 0.00018 -0.00298 -0.00280 3.77674

R31 2.57890 0.00022 0.00049 -0.00003 0.00046 2.57937

R32 2.56373 -0.00004 -0.00066 0.00080 0.00015 2.56388

R33 2.57974 0.00043 0.00098 0.00014 0.00112 2.58086

R34 3.79694 -0.00065 0.00024 -0.00247 -0.00223 3.79471

R35 2.77331 -0.00013 -0.00046 -0.00097 -0.00142 2.77189

R36 2.59737 0.00020 0.00053 0.00016 0.00069 2.59806

R37 2.81314 0.00004 -0.00002 0.00017 0.00015 2.81329

R38 2.73404 -0.00046 -0.00091 -0.00038 -0.00129 2.73275

R39 2.04314 -0.00005 -0.00001 -0.00013 -0.00014 2.04300

R40 2.58705 -0.00025 -0.00004 0.00019 0.00016 2.58721

R41 2.06253 -0.00008 -0.00001 -0.00002 -0.00004 2.06250

R42 2.06995 -0.00016 -0.00002 -0.00002 -0.00004 2.06991

R43 2.06995 -0.00016 -0.00002 -0.00002 -0.00004 2.06991

R44 2.06950 -0.00026 -0.00005 -0.00004 -0.00008 2.06942

R45 2.06950 -0.00026 -0.00005 -0.00004 -0.00008 2.06942

R46 2.06173 -0.00005 -0.00003 -0.00006 -0.00009 2.06165

R47 2.06950 -0.00026 -0.00005 -0.00004 -0.00008 2.06942

R48 2.06950 -0.00026 -0.00005 -0.00004 -0.00008 2.06942

R49 2.06173 -0.00005 -0.00003 -0.00006 -0.00009 2.06165

R50 2.06995 -0.00016 -0.00002 -0.00002 -0.00004 2.06991

R51 2.06995 -0.00016 -0.00002 -0.00002 -0.00004 2.06991

R52 2.06253 -0.00008 -0.00001 -0.00002 -0.00004 2.06250

A1 1.89297 -0.00004 -0.00012 0.00060 0.00048 1.89345

A2 2.20508 0.00004 -0.00005 0.00012 0.00008 2.20516

A3 2.18513 -0.00000 0.00017 -0.00073 -0.00056 2.18458

A4 1.90557 0.00021 0.00001 -0.00090 -0.00089 1.90468

A5 2.19268 -0.00004 -0.00081 0.00075 -0.00006 2.19262

A6 2.18493 -0.00017 0.00081 0.00015 0.00096 2.18589

A7 1.89700 -0.00040 0.00006 0.00043 0.00049 1.89749

A8 2.22309 0.00005 -0.00015 -0.00040 -0.00056 2.22253

A9 2.16309 0.00034 0.00009 -0.00003 0.00006 2.16316

A10 1.85046 0.00039 0.00008 0.00014 0.00022 1.85068

A11 2.17552 -0.00038 0.00035 0.00013 0.00048 2.17600

A12 2.25721 -0.00001 -0.00043 -0.00027 -0.00071 2.25650

A13 1.87877 -0.00017 -0.00002 -0.00028 -0.00030 1.87847

A14 2.18132 -0.00004 0.00029 -0.00027 0.00002 2.18135

A15 2.22309 0.00021 -0.00027 0.00054 0.00028 2.22337

A16 2.16765 0.00002 -0.00067 -0.00022 -0.00090 2.16676

A17 2.23152 -0.00017 0.00025 -0.00020 0.00005 2.23157

A18 2.16766 0.00006 -0.00020 -0.00041 -0.00061 2.16706

A19 1.88401 0.00011 -0.00005 0.00061 0.00056 1.88456

A20 1.91433 -0.00040 0.00005 -0.00137 -0.00131 1.91302

A21 2.18920 0.00014 0.00057 0.00021 0.00078 2.18999

A22 2.17965 0.00026 -0.00063 0.00116 0.00053 2.18018

A23 1.88400 0.00037 -0.00017 0.00113 0.00097 1.88497

A24 2.24778 -0.00014 -0.00018 -0.00014 -0.00032 2.24746

A25 2.15140 -0.00023 0.00035 -0.00100 -0.00064 2.15076

A26 1.85740 -0.00028 0.00014 -0.00049 -0.00035 1.85705

A27 2.15403 0.00015 0.00043 0.00021 0.00063 2.15466

A28 2.27176 0.00012 -0.00057 0.00029 -0.00028 2.27148

A29 1.88504 0.00020 0.00003 0.00012 0.00014 1.88518

A30 2.16489 -0.00009 0.00017 -0.00036 -0.00019 2.16470

A31 2.23326 -0.00011 -0.00020 0.00024 0.00005 2.23331

A32 2.16956 0.00000 0.00086 -0.00142 -0.00056 2.16900

A33 1.85740 -0.00028 0.00014 -0.00049 -0.00035 1.85705

A34 2.27176 0.00012 -0.00057 0.00029 -0.00028 2.27148

A35 2.15403 0.00015 0.00043 0.00021 0.00063 2.15466

A36 1.88504 0.00020 0.00003 0.00012 0.00014 1.88518

A37 2.23326 -0.00011 -0.00020 0.00024 0.00005 2.23331

A38 2.16489 -0.00009 0.00017 -0.00036 -0.00019 2.16470

A39 1.88401 0.00011 -0.00005 0.00061 0.00056 1.88456

A40 2.16766 0.00006 -0.00020 -0.00041 -0.00061 2.16706

A41 2.23152 -0.00017 0.00025 -0.00020 0.00005 2.23157

A42 1.91433 -0.00040 0.00005 -0.00137 -0.00131 1.91302

A43 2.18920 0.00014 0.00057 0.00021 0.00078 2.18999

A44 2.17965 0.00026 -0.00063 0.00116 0.00053 2.18018

A45 2.15140 -0.00023 0.00035 -0.00100 -0.00064 2.15076

A46 2.24778 -0.00014 -0.00018 -0.00014 -0.00032 2.24746

A47 1.88400 0.00037 -0.00017 0.00113 0.00097 1.88497

A48 2.16765 0.00002 -0.00067 -0.00022 -0.00090 2.16676

A49 1.90557 0.00021 0.00001 -0.00090 -0.00089 1.90468

A50 2.18493 -0.00017 0.00081 0.00015 0.00096 2.18589

A51 2.19268 -0.00004 -0.00081 0.00075 -0.00006 2.19262

A52 2.22309 0.00005 -0.00015 -0.00040 -0.00056 2.22253

A53 2.16309 0.00034 0.00009 -0.00003 0.00006 2.16316

A54 1.89700 -0.00040 0.00006 0.00043 0.00049 1.89749

A55 1.85046 0.00039 0.00008 0.00014 0.00022 1.85068

A56 2.17552 -0.00038 0.00035 0.00013 0.00048 2.17600

A57 2.25721 -0.00001 -0.00043 -0.00027 -0.00071 2.25650

A58 1.87877 -0.00017 -0.00002 -0.00028 -0.00030 1.87847

A59 2.22309 0.00021 -0.00027 0.00054 0.00028 2.22337

A60 2.18132 -0.00004 0.00029 -0.00027 0.00002 2.18135

A61 1.89297 -0.00004 -0.00012 0.00060 0.00048 1.89345

A62 2.20508 0.00004 -0.00005 0.00012 0.00008 2.20516

A63 2.18513 -0.00000 0.00017 -0.00073 -0.00056 2.18458

A64 2.16956 0.00000 0.00086 -0.00142 -0.00056 2.16900

A65 1.56998 0.00012 -0.00080 0.00047 -0.00034 1.56964

A66 1.57162 -0.00012 0.00080 -0.00047 0.00034 1.57195

A67 1.57162 -0.00012 0.00080 -0.00047 0.00034 1.57195

A68 1.56998 0.00012 -0.00080 0.00047 -0.00034 1.56964

A69 1.94289 0.00005 -0.00022 -0.00010 -0.00032 1.94257

A70 1.94045 0.00001 0.00002 -0.00004 -0.00002 1.94043

A71 1.94045 0.00001 0.00002 -0.00004 -0.00002 1.94043

A72 1.88984 -0.00005 0.00003 -0.00003 0.00000 1.88985

A73 1.88984 -0.00005 0.00003 -0.00003 0.00000 1.88985

A74 1.85722 0.00002 0.00012 0.00027 0.00038 1.85761

A75 1.93471 -0.00018 0.00004 -0.00037 -0.00033 1.93438

A76 1.93471 -0.00018 0.00004 -0.00037 -0.00033 1.93438

A77 1.94476 0.00017 -0.00035 0.00010 -0.00025 1.94451

A78 1.85679 0.00015 0.00021 0.00027 0.00048 1.85727

A79 1.89504 0.00002 0.00004 0.00021 0.00025 1.89529

A80 1.89504 0.00002 0.00004 0.00021 0.00025 1.89529

A81 1.93471 -0.00018 0.00004 -0.00037 -0.00033 1.93438

A82 1.93471 -0.00018 0.00004 -0.00037 -0.00033 1.93438

A83 1.94476 0.00017 -0.00035 0.00010 -0.00025 1.94451

A84 1.85679 0.00015 0.00021 0.00027 0.00048 1.85727

A85 1.89504 0.00002 0.00004 0.00021 0.00025 1.89529

A86 1.89504 0.00002 0.00004 0.00021 0.00025 1.89529

A87 1.94045 0.00001 0.00002 -0.00004 -0.00002 1.94043

A88 1.94045 0.00001 0.00002 -0.00004 -0.00002 1.94043

A89 1.94289 0.00005 -0.00022 -0.00010 -0.00032 1.94257

A90 1.85722 0.00002 0.00012 0.00027 0.00038 1.85761

A91 1.88984 -0.00005 0.00003 -0.00003 0.00000 1.88985

A92 1.88984 -0.00005 0.00003 -0.00003 0.00000 1.88985

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

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A96 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

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D2 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

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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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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

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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 1.03292 0.00002 0.00009 0.00014 0.00023 1.03315

D31 -1.03292 -0.00002 -0.00009 -0.00014 -0.00023 -1.03315

D32 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.10867 0.00002 0.00009 0.00014 0.00023 -2.10844

D34 2.10867 -0.00002 -0.00009 -0.00014 -0.00023 2.10844

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

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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

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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

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D57 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

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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 1.02897 -0.00002 0.00016 -0.00007 0.00009 1.02906

D64 -1.02897 0.00002 -0.00016 0.00007 -0.00009 -1.02906

D65 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

D66 -2.11262 -0.00002 0.00016 -0.00007 0.00009 -2.11253

D67 2.11262 0.00002 -0.00016 0.00007 -0.00009 2.11253

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 -2.11262 -0.00002 0.00016 -0.00007 0.00009 -2.11253

D80 2.11262 0.00002 -0.00016 0.00007 -0.00009 2.11253

D81 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D82 1.02897 -0.00002 0.00016 -0.00007 0.00009 1.02906

D83 -1.02897 0.00002 -0.00016 0.00007 -0.00009 -1.02906

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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D94 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D99 3.14159 -0.00000 0.00000 0.00000 0.00000 3.14159

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D106 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

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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

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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

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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 1.03292 0.00002 0.00009 0.00014 0.00023 1.03315

D126 -1.03292 -0.00002 -0.00009 -0.00014 -0.00023 -1.03315

D127 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

D128 -2.10867 0.00002 0.00009 0.00014 0.00023 -2.10844

D129 2.10867 -0.00002 -0.00009 -0.00014 -0.00023 2.10844

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 0.001032 0.000450 NO

RMS Force 0.000186 0.000300 YES

Maximum Displacement 0.002931 0.001800 NO

RMS Displacement 0.000728 0.001200 YES

Predicted change in Energy=-8.048152D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:36:15 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 -2.071170 -2.191560 0.000000

2 7 0 -0.745126 -1.864713 0.000000

3 6 0 -0.006655 -3.002877 0.000000

4 6 0 -0.915860 -4.153923 0.000000

5 6 0 -2.188156 -3.632929 0.000000

6 7 0 1.354328 -3.106769 0.000000

7 6 0 2.177240 -2.072646 0.000000

8 7 0 1.855024 -0.743745 0.000000

9 6 0 2.995908 0.003893 0.000000

10 6 0 4.167534 -0.936839 0.000000

11 6 0 3.654099 -2.184940 0.000000

12 7 0 -3.122912 -1.315057 0.000000

13 6 0 -4.167534 0.936839 0.000000

14 6 0 -3.654099 2.184940 0.000000

15 6 0 -2.177240 2.072646 0.000000

16 7 0 -1.855024 0.743745 0.000000

17 6 0 -2.995908 -0.003893 0.000000

18 7 0 -1.354328 3.106769 0.000000

19 7 0 0.745126 1.864713 0.000000

20 6 0 0.006655 3.002877 0.000000

21 6 0 0.915860 4.153923 0.000000

22 6 0 2.188156 3.632929 0.000000

23 6 0 2.071170 2.191560 0.000000

24 7 0 3.122912 1.315057 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.480119 -5.577456 0.000000

27 1 0 -3.121183 -4.179059 0.000000

28 6 0 5.582220 -0.483035 0.000000

29 1 0 4.189492 -3.124343 0.000000

30 6 0 -5.582220 0.483035 0.000000

31 1 0 -4.189492 3.124343 0.000000

32 6 0 0.480119 5.577456 0.000000

33 1 0 3.121183 4.179059 0.000000

34 1 0 -1.336404 -6.254205 0.000000

35 1 0 0.135859 -5.802751 0.877270

36 1 0 0.135859 -5.802751 -0.877270

37 1 0 5.791849 0.138442 0.876952

38 1 0 5.791849 0.138442 -0.876952

39 1 0 6.271708 -1.328516 0.000000

40 1 0 -5.791849 -0.138442 0.876952

41 1 0 -5.791849 -0.138442 -0.876952

42 1 0 -6.271708 1.328516 0.000000

43 1 0 -0.135859 5.802751 0.877270

44 1 0 -0.135859 5.802751 -0.877270

45 1 0 1.336404 6.254205 0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.365732 0.000000

3 C 2.218211 1.356745 0.000000

4 C 2.277193 2.295568 1.466820 0.000000

5 C 1.446108 2.282307 2.270664 1.374835 0.000000

6 N 3.545651 2.439346 1.364942 2.500056 3.581346

7 C 4.250073 2.929753 2.373757 3.728133 4.635856

8 N 4.184635 2.831492 2.927375 4.393986 4.969375

9 C 5.522254 4.181748 4.249241 5.708709 6.332535

10 C 6.363628 4.999518 4.657507 6.015856 6.903891

11 C 5.725272 4.410864 3.751018 4.976084 6.019021

12 N 1.369094 2.440489 3.543980 3.595863 2.499259

13 C 3.765850 4.422847 5.730120 6.040632 4.980031

14 C 4.653968 4.986162 6.341710 6.905007 5.999715

15 C 4.265525 4.189719 5.520178 6.353049 5.705585

16 N 2.943253 2.834771 4.177756 4.986900 4.389334

17 C 2.375085 2.920389 4.234329 4.642127 3.717844

18 N 5.346603 5.008669 6.256517 7.273919 6.791082

19 N 4.938104 4.016150 4.925302 6.243624 6.231228

20 C 5.594599 4.925302 6.005769 7.216011 6.989357

21 C 7.013380 6.243624 7.216011 8.507378 8.382719

22 C 7.215714 6.231228 6.989357 8.382719 8.482028

23 C 6.030815 4.938104 5.594599 7.013380 7.215714

24 N 6.266965 5.007260 5.332799 6.798634 7.258789

25 Zn 3.015407 2.008075 3.002884 4.253689 4.241014

26 C 3.741087 3.722189 2.617752 1.488730 2.588161

27 H 2.247816 3.316903 3.329218 2.205466 1.081109

28 C 7.841775 6.476445 6.130671 7.463274 8.384544

29 H 6.329768 5.092849 4.197904 5.208133 6.397894

30 C 4.413722 5.376747 6.575600 6.578472 5.334869

31 H 5.722422 6.062535 7.418824 7.980590 7.047416

32 C 8.177206 7.542354 8.594130 9.830996 9.589102

33 H 8.218596 7.174644 7.833490 9.259390 9.445435

34 H 4.128554 4.429136 3.512743 2.141971 2.756187

35 H 4.322184 4.129635 2.937551 2.143444 3.298299

36 H 4.322184 4.129635 2.937551 2.143444 3.298299

37 H 8.247728 6.893019 6.652787 8.011666 8.869767

38 H 8.247728 6.893019 6.652787 8.011666 8.869767

39 H 8.387398 7.037290 6.497793 7.722956 8.768102

40 H 4.339101 5.405412 6.514792 6.377178 5.095791

41 H 4.339101 5.405412 6.514792 6.377178 5.095791

42 H 5.480461 6.382775 7.616551 7.664348 6.425833

43 H 8.271883 7.741499 8.850163 10.025635 9.696060

44 H 8.271883 7.741499 8.850163 10.025635 9.696060

45 H 9.107277 8.381502 9.354003 10.649028 10.496567

6 7 8 9 10

6 N 0.000000

7 C 1.321588 0.000000

8 N 2.415488 1.367406 0.000000

9 C 3.517244 2.232091 1.364030 0.000000

10 C 3.552848 2.291578 2.320558 1.502559 0.000000

11 C 2.477643 1.481122 2.305149 2.285652 1.349583

12 N 4.822438 5.354021 5.010613 6.259360 7.300250

13 C 6.844101 7.022332 6.252645 7.223939 8.543070

14 C 7.286050 7.220217 6.239201 6.998539 8.421606

15 C 6.268836 6.012065 4.918456 5.571462 7.022332

16 N 5.012624 4.918456 3.997134 4.907028 6.252645

17 C 5.343444 5.571462 4.907028 5.991821 7.223939

18 N 6.778265 6.268836 5.012624 5.343444 6.844101

19 N 5.008669 4.189719 2.834771 2.920389 4.422847

20 C 6.256517 5.520178 4.177756 4.234329 5.730120

21 C 7.273919 6.353049 4.986900 4.642127 6.040632

22 C 6.791082 5.705585 4.389334 3.717844 4.980031

23 C 5.346603 4.265525 2.943253 2.375085 3.765850

24 N 4.762399 3.517219 2.417893 1.317301 2.482392

25 Zn 3.389132 3.006033 1.998567 2.995910 4.271535

26 C 3.077253 4.398324 5.368208 6.575274 6.567801

27 H 4.602174 5.701777 6.046819 7.410526 7.977305

28 C 4.975847 3.757759 3.736303 2.631751 1.485690

29 H 2.835218 2.270512 3.334215 3.348209 2.187615

30 C 7.810403 8.169500 7.537745 8.591500 9.852602

31 H 8.340305 8.218513 7.176230 7.833720 9.291560

32 C 8.728116 7.836088 6.468999 6.115047 7.485524

33 H 7.497004 6.322566 5.083026 4.177045 5.221806

34 H 4.140819 5.461788 6.367918 7.611354 7.652955

35 H 3.085869 4.341719 5.414672 6.531968 6.379743

36 H 3.085869 4.341719 5.414672 6.531968 6.379743

37 H 5.567049 4.327049 4.128667 2.933332 2.136275

38 H 5.567049 4.327049 4.128667 2.933332 2.136275

39 H 5.229035 4.161538 4.455227 3.536407 2.140317

40 H 7.787673 8.247216 7.720758 8.832552 10.029746

41 H 7.787673 8.247216 7.720758 8.832552 10.029746

42 H 8.822027 9.107832 8.386777 9.361801 10.682210

43 H 9.075782 8.254811 6.898538 6.648633 8.044306

44 H 9.075782 8.254811 6.898538 6.648633 8.044306

45 H 9.360991 8.369196 7.017141 6.466865 7.728286

11 12 13 14 15

11 C 0.000000

12 N 6.832610 0.000000

13 C 8.421606 2.482392 0.000000

14 C 8.515022 3.540076 1.349583 0.000000

15 C 7.220217 3.517219 2.291578 1.481122 0.000000

16 N 6.239201 2.417893 2.320558 2.305149 1.367406

17 C 6.998539 1.317301 1.502559 2.285652 2.232091

18 N 7.286050 4.762399 3.552848 2.477643 1.321588

19 N 4.986162 5.007260 4.999518 4.410864 2.929753

20 C 6.341710 5.332799 4.657507 3.751018 2.373757

21 C 6.905007 6.798634 6.015856 4.976084 3.728133

22 C 5.999715 7.258789 6.903891 6.019021 4.635856

23 C 4.653968 6.266965 6.363628 5.725272 4.250073

24 N 3.540076 6.777007 7.300250 6.832610 5.354021

25 Zn 4.257511 3.388503 4.271535 4.257511 3.006033

26 C 5.347983 5.015217 7.485524 8.386235 7.836088

27 H 7.062645 2.864002 5.221806 6.386273 6.322566

28 C 2.571796 8.744804 9.852602 9.613932 8.169500

29 H 1.081260 7.532912 9.291560 9.471557 8.218513

30 C 9.613932 3.046529 1.485690 2.571796 3.757759

31 H 9.471557 4.565728 2.187615 1.081260 2.270512

32 C 8.386235 7.777440 6.567801 5.347983 4.398324

33 H 6.386273 8.317093 7.977305 7.062645 5.701777

34 H 6.439257 5.252312 7.728286 8.751621 8.369196

35 H 5.122126 5.615032 8.044306 8.884626 8.254811

36 H 5.122126 5.615032 8.044306 8.884626 8.254811

37 H 3.276755 9.074947 10.029746 9.704799 8.247216

38 H 3.276755 9.074947 10.029746 9.704799 8.247216

39 H 2.754149 9.394629 10.682210 10.529292 9.107832

40 H 9.704799 3.045767 2.136275 3.276755 4.327049

41 H 9.704799 3.045767 2.136275 3.276755 4.327049

42 H 10.529292 4.111374 2.140317 2.754149 4.161538

43 H 8.884626 7.768867 6.379743 5.122126 4.341719

44 H 8.884626 7.768867 6.379743 5.122126 4.341719

45 H 8.751621 8.785171 7.652955 6.439257 5.461788

16 17 18 19 20

16 N 0.000000

17 C 1.364030 0.000000

18 N 2.415488 3.517244 0.000000

19 N 2.831492 4.181748 2.439346 0.000000

20 C 2.927375 4.249241 1.364942 1.356745 0.000000

21 C 4.393986 5.708709 2.500056 2.295568 1.466820

22 C 4.969375 6.332535 3.581346 2.282307 2.270664

23 C 4.184635 5.522254 3.545651 1.365732 2.218211

24 N 5.010613 6.259360 4.822438 2.440489 3.543980

25 Zn 1.998567 2.995910 3.389132 2.008075 3.002884

26 C 6.468999 6.115047 8.728116 7.542354 8.594130

27 H 5.083026 4.177045 7.497004 7.174644 7.833490

28 C 7.537745 8.591500 7.810403 5.376747 6.575600

29 H 7.176230 7.833720 8.340305 6.062535 7.418824

30 C 3.736303 2.631751 4.975847 6.476445 6.130671

31 H 3.334215 3.348209 2.835218 5.092849 4.197904

32 C 5.368208 6.575274 3.077253 3.722189 2.617752

33 H 6.046819 7.410526 4.602174 3.316903 3.329218

34 H 7.017141 6.466865 9.360991 8.381502 9.354003

35 H 6.898538 6.648633 9.075782 7.741499 8.850163

36 H 6.898538 6.648633 9.075782 7.741499 8.850163

37 H 7.720758 8.832552 7.787673 5.405412 6.514792

38 H 7.720758 8.832552 7.787673 5.405412 6.514792

39 H 8.386777 9.361801 8.822027 6.382775 7.616551

40 H 4.128667 2.933332 5.567049 6.893019 6.652787

41 H 4.128667 2.933332 5.567049 6.893019 6.652787

42 H 4.455227 3.536407 5.229035 7.037290 6.497793

43 H 5.414672 6.531968 3.085869 4.129635 2.937551

44 H 5.414672 6.531968 3.085869 4.129635 2.937551

45 H 6.367918 7.611354 4.140819 4.429136 3.512743

21 22 23 24 25

21 C 0.000000

22 C 1.374835 0.000000

23 C 2.277193 1.446108 0.000000

24 N 3.595863 2.499259 1.369094 0.000000

25 Zn 4.253689 4.241014 3.015407 3.388503 0.000000

26 C 9.830996 9.589102 8.177206 7.777440 5.598083

27 H 9.259390 9.445435 8.218596 8.317093 5.215967

28 C 6.578472 5.334869 4.413722 3.046529 5.603080

29 H 7.980590 7.047416 5.722422 4.565728 5.226218

30 C 7.463274 8.384544 7.841775 8.744804 5.603080

31 H 5.208133 6.397894 6.329768 7.532912 5.226218

32 C 1.488730 2.588161 3.741087 5.015217 5.598083

33 H 2.205466 1.081109 2.247816 2.864002 5.215967

34 H 10.649028 10.496567 9.107277 8.785171 6.395393

35 H 10.025635 9.696060 8.271883 7.768867 5.870263

36 H 10.025635 9.696060 8.271883 7.768867 5.870263

37 H 6.377178 5.095791 4.339101 3.045767 5.859499

38 H 6.377178 5.095791 4.339101 3.045767 5.859499

39 H 7.664348 6.425833 5.480461 4.111374 6.410871

40 H 8.011666 8.869767 8.247728 9.074947 5.859499

41 H 8.011666 8.869767 8.247728 9.074947 5.859499

42 H 7.722956 8.768102 8.387398 9.394629 6.410871

43 H 2.143444 3.298299 4.322184 5.615032 5.870263

44 H 2.143444 3.298299 4.322184 5.615032 5.870263

45 H 2.141971 2.756187 4.128554 5.252312 6.395393

26 27 28 29 30

26 C 0.000000

27 H 2.988434 0.000000

28 C 7.918654 9.455677 0.000000

29 H 5.274753 7.386365 2.986001 0.000000

30 C 7.922184 5.271795 11.206161 10.416311 0.000000

31 H 9.459427 7.381122 10.416311 10.452437 2.986001

32 C 11.196166 10.399950 7.922184 9.459427 7.918654

33 H 10.399950 10.431935 5.271795 7.381122 9.455677

34 H 1.091427 2.737091 9.009648 6.350713 7.963502

35 H 1.095349 3.743568 7.663670 4.937146 8.542666

36 H 1.095349 3.743568 7.663670 4.937146 8.542666

37 H 8.531009 9.942434 1.095090 3.739299 11.413030

38 H 8.531009 9.942434 1.095090 3.739299 11.413030

39 H 7.977509 9.815905 1.090976 2.749658 11.991552

40 H 7.652869 4.922203 11.413030 10.455229 1.095090

41 H 7.652869 4.922203 11.413030 10.455229 1.095090

42 H 9.013043 6.345012 11.991552 11.369461 1.090976

43 H 11.419161 10.455539 8.542666 9.958477 7.663670

44 H 11.419161 10.455539 8.542666 9.958477 7.663670

45 H 11.970294 11.345619 7.963502 9.802921 9.009648

31 32 33 34 35

31 H 0.000000

32 C 5.274753 0.000000

33 H 7.386365 2.988434 0.000000

34 H 9.802921 11.970294 11.345619 0.000000

35 H 9.958477 11.419161 10.455539 1.772278 0.000000

36 H 9.958477 11.419161 10.455539 1.772278 1.754540

37 H 10.455229 7.652869 4.922203 9.614934 8.202926

38 H 10.455229 7.652869 4.922203 9.614934 8.388402

39 H 11.369461 9.013043 6.345012 9.063430 7.644411

40 H 3.739299 8.531009 9.942434 7.617256 8.198910

41 H 3.739299 8.531009 9.942434 7.617256 8.384475

42 H 2.749658 7.977509 9.815905 9.047368 9.627122

43 H 4.937146 1.095349 3.743568 12.148296 11.608683

44 H 4.937146 1.095349 3.743568 12.148296 11.740525

45 H 6.350713 1.091427 2.737091 12.790786 12.148296

36 37 38 39 40

36 H 0.000000

37 H 8.388402 0.000000

38 H 8.202926 1.753903 0.000000

39 H 7.644411 1.775182 1.775182 0.000000

40 H 8.384475 11.587007 11.718998 12.153794 0.000000

41 H 8.198910 11.718998 11.587007 12.153794 1.753903

42 H 9.627122 12.153794 12.153794 12.821742 1.775182

43 H 11.740525 8.198910 8.384475 9.627122 8.202926

44 H 11.608683 8.384475 8.198910 9.627122 8.388402

45 H 12.148296 7.617256 7.617256 9.047368 9.614934

41 42 43 44 45

41 H 0.000000

42 H 1.775182 0.000000

43 H 8.388402 7.644411 0.000000

44 H 8.202926 7.644411 1.754540 0.000000

45 H 9.614934 9.063430 1.772278 1.772278 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=0 Diff= 2.04D-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 2.943870 -0.652924 0.000000

2 7 0 1.982825 0.317444 0.000000

3 6 0 2.580698 1.535355 0.000000

4 6 0 4.035208 1.345723 0.000000

5 6 0 4.240992 -0.013625 0.000000

6 7 0 1.971414 2.756764 0.000000

7 6 0 0.661540 2.932336 0.000000

8 7 0 -0.313657 1.973801 0.000000

9 6 0 -1.540831 2.569303 0.000000

10 6 0 -1.334703 4.057657 0.000000

11 6 0 0.000000 4.257511 0.000000

12 7 0 2.731343 -2.005422 0.000000

13 6 0 1.334703 -4.057657 0.000000

14 6 0 -0.000000 -4.257511 0.000000

15 6 0 -0.661540 -2.932336 0.000000

16 7 0 0.313657 -1.973801 0.000000

17 6 0 1.540831 -2.569303 0.000000

18 7 0 -1.971414 -2.756764 0.000000

19 7 0 -1.982825 -0.317444 0.000000

20 6 0 -2.580698 -1.535355 0.000000

21 6 0 -4.035208 -1.345723 0.000000

22 6 0 -4.240992 0.013625 0.000000

23 6 0 -2.943870 0.652924 0.000000

24 7 0 -2.731343 2.005422 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 5.033365 2.450259 0.000000

27 1 0 5.188546 -0.534143 0.000000

28 6 0 -2.450201 5.038951 0.000000

29 1 0 0.531501 5.199122 0.000000

30 6 0 2.450201 -5.038951 0.000000

31 1 0 -0.531501 -5.199122 0.000000

32 6 0 -5.033365 -2.450259 0.000000

33 1 0 -5.188546 0.534143 0.000000

34 1 0 6.053641 2.062639 0.000000

35 1 0 4.910612 3.094555 0.877270

36 1 0 4.910612 3.094555 -0.877270

37 1 0 -3.091178 4.899929 0.876952

38 1 0 -3.091178 4.899929 -0.876952

39 1 0 -2.078392 6.064615 0.000000

40 1 0 3.091178 -4.899929 0.876952

41 1 0 3.091178 -4.899929 -0.876952

42 1 0 2.078392 -6.064615 0.000000

43 1 0 -4.910612 -3.094555 0.877270

44 1 0 -4.910612 -3.094555 -0.877270

45 1 0 -6.053641 -2.062639 0.000000

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

Rotational constants (GHZ): 0.1829510 0.1820692 0.0914594

Leave Link 202 at Tue Sep 17 14:36:15 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 101 beta electrons

nuclear repulsion energy 2762.2526919161 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= -0.1142189378 Hartrees.

Nuclear repulsion after empirical dispersion term = 2762.1384729783 Hartrees.

No density basis found on file 724.

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Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 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 = 3594

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.16D-07

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 248

GePol: Fraction of low-weight points (<1% of avg) = 6.90%

GePol: Cavity surface area = 378.450 Ang\*\*2

GePol: Cavity volume = 378.157 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0106940942 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2762.1277788842 Hartrees.

Leave Link 301 at Tue Sep 17 14:36:15 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= 15327 LenP2D= 41276.

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 14:36:16 2019, MaxMem= 2415919104 cpu: 13.0

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:36:16 2019, MaxMem= 2415919104 cpu: 1.2

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

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= 0.000000 -0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000052 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)

(BU) (AG) (BU) (AG) (BU) (AG) (BU) (AG) (BU) (AG)

(BU) (AG) (BU) (AG) (BU) (AG) (BU) (AG) (AG) (BU)

(BU) (AG) (AG) (BU) (BU) (AG) (AG) (BU) (BU) (AG)

(AG) (BU) (BU) (AG) (AG) (BU) (BU) (AG) (AG) (AG)

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The electronic state of the initial guess is 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0178 S= 1.0059

Leave Link 401 at Tue Sep 17 14:36:17 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= 38750508.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.11D-15 for 3585.

Iteration 1 A\*A^-1 deviation from orthogonality is 5.55D-15 for 3591 1330.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.22D-15 for 3585.

Iteration 1 A^-1\*A deviation from orthogonality is 4.16D-12 for 1743 1741.

E= -1275.84275656110

DIIS: error= 1.47D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.84275656110 IErMin= 1 ErrMin= 1.47D-04

ErrMax= 1.47D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.05D-05 BMatP= 2.05D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.47D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.304 Goal= None Shift= 0.000

Gap= 0.393 Goal= None Shift= 0.000

RMSDP=5.74D-06 MaxDP=2.28D-04 OVMax= 8.23D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 5.73D-06 CP: 1.00D+00

E= -1275.84276133378 Delta-E= -0.000004772683 Rises=F Damp=F

DIIS: error= 5.02D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84276133378 IErMin= 2 ErrMin= 5.02D-05

ErrMax= 5.02D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.46D-07 BMatP= 2.05D-05

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

Coeff-Com: 0.404D-01 0.960D+00

Coeff: 0.404D-01 0.960D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.69D-06 MaxDP=6.86D-05 DE=-4.77D-06 OVMax= 6.67D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.67D-06 CP: 1.00D+00 1.04D+00

E= -1275.84276123207 Delta-E= 0.000000101714 Rises=F Damp=F

DIIS: error= 6.61D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1275.84276133378 IErMin= 2 ErrMin= 5.02D-05

ErrMax= 6.61D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.87D-06 BMatP= 9.46D-07

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

Coeff-Com: -0.924D-02 0.596D+00 0.413D+00

Coeff: -0.924D-02 0.596D+00 0.413D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=9.36D-07 MaxDP=4.33D-05 DE= 1.02D-07 OVMax= 1.75D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 6.57D-07 CP: 1.00D+00 1.07D+00 6.13D-01

E= -1275.84276158173 Delta-E= -0.000000349656 Rises=F Damp=F

DIIS: error= 7.57D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84276158173 IErMin= 4 ErrMin= 7.57D-06

ErrMax= 7.57D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.16D-08 BMatP= 9.46D-07

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

Coeff-Com: -0.712D-02 0.193D+00 0.188D+00 0.626D+00

Coeff: -0.712D-02 0.193D+00 0.188D+00 0.626D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.87D-07 MaxDP=2.09D-05 DE=-3.50D-07 OVMax= 2.45D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.88D-07 CP: 1.00D+00 1.07D+00 7.56D-01 1.13D+00

E= -1275.84276160928 Delta-E= -0.000000027555 Rises=F Damp=F

DIIS: error= 7.35D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84276160928 IErMin= 5 ErrMin= 7.35D-06

ErrMax= 7.35D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.06D-08 BMatP= 6.16D-08

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

Coeff-Com: -0.212D-02 0.265D-01 0.434D-01 0.369D+00 0.564D+00

Coeff: -0.212D-02 0.265D-01 0.434D-01 0.369D+00 0.564D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.88D-07 MaxDP=1.30D-05 DE=-2.76D-08 OVMax= 2.01D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.24D-07 CP: 1.00D+00 1.08D+00 8.18D-01 1.46D+00 1.30D+00

E= -1275.84276162516 Delta-E= -0.000000015879 Rises=F Damp=F

DIIS: error= 5.41D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84276162516 IErMin= 6 ErrMin= 5.41D-06

ErrMax= 5.41D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.85D-09 BMatP= 2.06D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.231D-02-0.618D-01-0.673D-01-0.186D+00-0.244D-01 0.134D+01

Coeff: 0.231D-02-0.618D-01-0.673D-01-0.186D+00-0.244D-01 0.134D+01

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=5.46D-07 MaxDP=2.84D-05 DE=-1.59D-08 OVMax= 4.11D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 9.90D-08 CP: 1.00D+00 1.10D+00 9.72D-01 1.99D+00 2.27D+00

CP: 2.01D+00

E= -1275.84276164561 Delta-E= -0.000000020449 Rises=F Damp=F

DIIS: error= 3.63D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84276164561 IErMin= 7 ErrMin= 3.63D-06

ErrMax= 3.63D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.61D-09 BMatP= 4.85D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.276D-02-0.571D-01-0.747D-01-0.323D+00-0.348D+00 0.878D+00

Coeff-Com: 0.922D+00

Coeff: 0.276D-02-0.571D-01-0.747D-01-0.323D+00-0.348D+00 0.878D+00

Coeff: 0.922D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=5.28D-07 MaxDP=2.55D-05 DE=-2.04D-08 OVMax= 3.94D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 8.98D-08 CP: 1.00D+00 1.11D+00 1.11D+00 2.51D+00 3.00D+00

CP: 3.00D+00 1.66D+00

E= -1275.84276165818 Delta-E= -0.000000012567 Rises=F Damp=F

DIIS: error= 2.34D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84276165818 IErMin= 8 ErrMin= 2.34D-06

ErrMax= 2.34D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.59D-09 BMatP= 3.61D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.132D-03 0.225D-01 0.837D-02-0.325D-01-0.201D+00-0.501D+00

Coeff-Com: 0.706D+00 0.999D+00

Coeff: -0.132D-03 0.225D-01 0.837D-02-0.325D-01-0.201D+00-0.501D+00

Coeff: 0.706D+00 0.999D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.69D-07 MaxDP=2.42D-05 DE=-1.26D-08 OVMax= 3.61D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.04D-07 CP: 1.00D+00 1.12D+00 1.23D+00 2.94D+00 3.00D+00

CP: 3.00D+00 2.65D+00 3.00D+00

E= -1275.84276166348 Delta-E= -0.000000005306 Rises=F Damp=F

DIIS: error= 1.02D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84276166348 IErMin= 9 ErrMin= 1.02D-06

ErrMax= 1.02D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.23D-10 BMatP= 1.59D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.646D-03 0.230D-01 0.165D-01 0.463D-01-0.193D-01-0.439D+00

Coeff-Com: 0.166D+00 0.508D+00 0.699D+00

Coeff: -0.646D-03 0.230D-01 0.165D-01 0.463D-01-0.193D-01-0.439D+00

Coeff: 0.166D+00 0.508D+00 0.699D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.26D-07 MaxDP=6.38D-06 DE=-5.31D-09 OVMax= 9.51D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 7.30D-08 CP: 1.00D+00 1.13D+00 1.27D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.96D+00 3.00D+00 1.24D+00

E= -1275.84276166410 Delta-E= -0.000000000616 Rises=F Damp=F

DIIS: error= 6.01D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84276166410 IErMin=10 ErrMin= 6.01D-07

ErrMax= 6.01D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.28D-10 BMatP= 4.23D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.315D-03 0.399D-02 0.501D-02 0.470D-01 0.932D-01-0.537D-01

Coeff-Com: -0.217D+00-0.852D-01 0.406D+00 0.802D+00

Coeff: -0.315D-03 0.399D-02 0.501D-02 0.470D-01 0.932D-01-0.537D-01

Coeff: -0.217D+00-0.852D-01 0.406D+00 0.802D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.83D-08 MaxDP=3.02D-06 DE=-6.16D-10 OVMax= 3.57D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 2.53D-08 CP: 1.00D+00 1.13D+00 1.28D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.34D+00 1.41D+00

E= -1275.84276166426 Delta-E= -0.000000000158 Rises=F Damp=F

DIIS: error= 3.09D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84276166426 IErMin=11 ErrMin= 3.09D-07

ErrMax= 3.09D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.89D-11 BMatP= 1.28D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.274D-04-0.433D-02-0.240D-02 0.699D-02 0.414D-01 0.864D-01

Coeff-Com: -0.138D+00-0.132D+00-0.921D-01 0.422D+00 0.812D+00

Coeff: 0.274D-04-0.433D-02-0.240D-02 0.699D-02 0.414D-01 0.864D-01

Coeff: -0.138D+00-0.132D+00-0.921D-01 0.422D+00 0.812D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.06D-08 MaxDP=1.69D-06 DE=-1.58D-10 OVMax= 2.24D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 9.13D-09 CP: 1.00D+00 1.13D+00 1.28D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.39D+00 1.72D+00

CP: 1.39D+00

E= -1275.84276166432 Delta-E= -0.000000000064 Rises=F Damp=F

DIIS: error= 1.20D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84276166432 IErMin=12 ErrMin= 1.20D-07

ErrMax= 1.20D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.71D-11 BMatP= 4.89D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.106D-03-0.377D-02-0.275D-02-0.944D-02-0.359D-02 0.719D-01

Coeff-Com: -0.279D-01-0.471D-01-0.221D+00 0.636D-01 0.511D+00 0.669D+00

Coeff: 0.106D-03-0.377D-02-0.275D-02-0.944D-02-0.359D-02 0.719D-01

Coeff: -0.279D-01-0.471D-01-0.221D+00 0.636D-01 0.511D+00 0.669D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.87D-08 MaxDP=1.08D-06 DE=-6.37D-11 OVMax= 1.44D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 3.83D-09 CP: 1.00D+00 1.13D+00 1.29D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.43D+00 1.89D+00

CP: 1.68D+00 1.21D+00

E= -1275.84276166433 Delta-E= -0.000000000013 Rises=F Damp=F

DIIS: error= 6.41D-08 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84276166433 IErMin=13 ErrMin= 6.41D-08

ErrMax= 6.41D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.45D-12 BMatP= 1.71D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.303D-04 0.187D-03-0.117D-03-0.520D-02-0.152D-01-0.300D-02

Coeff-Com: 0.277D-01 0.358D-01-0.660D-01-0.792D-01-0.873D-01 0.179D+00

Coeff-Com: 0.101D+01

Coeff: 0.303D-04 0.187D-03-0.117D-03-0.520D-02-0.152D-01-0.300D-02

Coeff: 0.277D-01 0.358D-01-0.660D-01-0.792D-01-0.873D-01 0.179D+00

Coeff: 0.101D+01

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.34D-08 MaxDP=7.08D-07 DE=-1.32D-11 OVMax= 1.04D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 2.19D-09 CP: 1.00D+00 1.13D+00 1.29D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.46D+00 2.02D+00

CP: 1.83D+00 1.50D+00 1.54D+00

E= -1275.84276166433 Delta-E= 0.000000000005 Rises=F Damp=F

DIIS: error= 1.98D-08 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=13 EnMin= -1275.84276166433 IErMin=14 ErrMin= 1.98D-08

ErrMax= 1.98D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.34D-13 BMatP= 2.45D-12

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.468D-05 0.701D-03 0.274D-03-0.902D-03-0.603D-02-0.139D-01

Coeff-Com: 0.164D-01 0.273D-01 0.574D-02-0.438D-01-0.126D+00-0.386D-01

Coeff-Com: 0.438D+00 0.740D+00

Coeff: -0.468D-05 0.701D-03 0.274D-03-0.902D-03-0.603D-02-0.139D-01

Coeff: 0.164D-01 0.273D-01 0.574D-02-0.438D-01-0.126D+00-0.386D-01

Coeff: 0.438D+00 0.740D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.44D-09 MaxDP=1.74D-07 DE= 4.55D-12 OVMax= 2.61D-06

Error on total polarization charges = 0.06475

SCF Done: E(UB3LYP) = -1275.84276166 A.U. after 14 cycles

NFock= 14 Conv=0.34D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0177 S= 1.0059

<L.S>= 0.000000000000E+00

KE= 1.320809175249D+03 PE=-8.576218782582D+03 EE= 3.217439066784D+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 2.0177, after 2.0002

Leave Link 502 at Tue Sep 17 14:37:31 2019, MaxMem= 2415919104 cpu: 1287.8

(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= 15327 LenP2D= 41276.

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 14:37:35 2019, MaxMem= 2415919104 cpu: 74.6

(Enter /home/blab/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Tue Sep 17 14:37:35 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 14:37:45 2019, MaxMem= 2415919104 cpu: 177.5

(Enter /home/blab/g09/l716.exe)

Dipole =-1.97175609D-13-7.99360578D-15 0.00000000D+00

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000558634 0.000058385 -0.000000000

2 7 -0.000080875 -0.000134017 0.000000000

3 6 0.000702400 0.000077764 0.000000000

4 6 -0.000641986 0.000295956 0.000000000

5 6 0.000047463 -0.000104390 0.000000000

6 7 0.000225169 0.000517645 0.000000000

7 6 -0.000269447 -0.000458291 -0.000000000

8 7 -0.000481009 0.000255409 -0.000000000

9 6 0.000072787 0.000685687 0.000000000

10 6 0.000553356 -0.000110164 -0.000000000

11 6 0.000144840 0.000225600 -0.000000000

12 7 0.000438205 0.000667741 0.000000000

13 6 -0.000553356 0.000110164 0.000000000

14 6 -0.000144840 -0.000225600 -0.000000000

15 6 0.000269447 0.000458291 -0.000000000

16 7 0.000481009 -0.000255409 -0.000000000

17 6 -0.000072787 -0.000685687 0.000000000

18 7 -0.000225169 -0.000517645 0.000000000

19 7 0.000080875 0.000134017 -0.000000000

20 6 -0.000702400 -0.000077764 0.000000000

21 6 0.000641986 -0.000295956 0.000000000

22 6 -0.000047463 0.000104390 0.000000000

23 6 0.000558634 -0.000058385 0.000000000

24 7 -0.000438205 -0.000667741 -0.000000000

25 30 -0.000000000 -0.000000000 0.000000000

26 6 0.000265592 0.000035765 -0.000000000

27 1 -0.000042662 0.000091577 -0.000000000

28 6 0.000063959 0.000146746 -0.000000000

29 1 -0.000039391 0.000073128 0.000000000

30 6 -0.000063959 -0.000146746 -0.000000000

31 1 0.000039391 -0.000073128 0.000000000

32 6 -0.000265592 -0.000035765 0.000000000

33 1 0.000042662 -0.000091577 -0.000000000

34 1 0.000093657 -0.000006199 -0.000000000

35 1 -0.000099300 -0.000001209 -0.000118458

36 1 -0.000099300 -0.000001209 0.000118458

37 1 -0.000115353 -0.000168598 -0.000155425

38 1 -0.000115353 -0.000168598 0.000155425

39 1 0.000054479 0.000075800 0.000000000

40 1 0.000115353 0.000168598 -0.000155425

41 1 0.000115353 0.000168598 0.000155425

42 1 -0.000054479 -0.000075800 -0.000000000

43 1 0.000099300 0.000001209 -0.000118458

44 1 0.000099300 0.000001209 0.000118458

45 1 -0.000093657 0.000006199 -0.000000000

-------------------------------------------------------------------

Cartesian Forces: Max 0.000702400 RMS 0.000245414

Leave Link 716 at Tue Sep 17 14:37:45 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 0.000809347 RMS 0.000134625

Search for a local minimum.

Step number 28 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 12 13 14 15

16 17 18 19 20

21 22 23 24 25

26 27 28

DE= -8.16D-06 DEPred=-8.05D-06 R= 1.01D+00

TightC=F SS= 1.41D+00 RLast= 8.11D-03 DXNew= 1.2880D-01 2.4339D-02

Trust test= 1.01D+00 RLast= 8.11D-03 DXMaxT set to 7.66D-02

ITU= 1 1 -1 1 -1 -1 1 0 0 1 -1 -1 1 1 -1 1 1 1 -1 0

ITU= 1 -1 1 1 1 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01335

Eigenvalues --- 0.01337 0.01346 0.01347 0.01604 0.01623

Eigenvalues --- 0.01631 0.01640 0.01774 0.01793 0.01809

Eigenvalues --- 0.01823 0.01890 0.01910 0.01939 0.01950

Eigenvalues --- 0.01997 0.02000 0.02045 0.02047 0.02070

Eigenvalues --- 0.02087 0.02103 0.02110 0.02115 0.02205

Eigenvalues --- 0.02312 0.02316 0.02351 0.02372 0.04737

Eigenvalues --- 0.06564 0.07199 0.07199 0.07200 0.07200

Eigenvalues --- 0.07315 0.07388 0.07411 0.08954 0.12598

Eigenvalues --- 0.14427 0.14498 0.14501 0.14794 0.14955

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16029 0.16260 0.16395 0.16588 0.17999

Eigenvalues --- 0.19990 0.20698 0.22057 0.22089 0.23497

Eigenvalues --- 0.23842 0.23854 0.24576 0.24934 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25335 0.26288 0.28008 0.29671 0.32255

Eigenvalues --- 0.32861 0.33187 0.33196 0.33282 0.33282

Eigenvalues --- 0.33597 0.33709 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33724 0.33724 0.34154 0.34382

Eigenvalues --- 0.34437 0.34437 0.34479 0.35555 0.35564

Eigenvalues --- 0.35612 0.35682 0.35682 0.35692 0.36347

Eigenvalues --- 0.37464 0.39163 0.41637 0.41812 0.42523

Eigenvalues --- 0.46196 0.48964 0.48976 0.49984 0.51136

Eigenvalues --- 0.51358 0.51361 0.52580 0.53495 0.54021

Eigenvalues --- 0.54029 0.56318 0.56326 0.59306

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 1.01580 -0.60665 0.12265 -0.03156 -0.06120

DIIS coeff's: 0.07276 0.30569 0.02266 0.06996 0.08989

Cosine: 0.772 > 0.000

Length: 1.176

GDIIS step was calculated using 10 of the last 28 vectors.

Iteration 1 RMS(Cart)= 0.00130548 RMS(Int)= 0.00000080

Iteration 2 RMS(Cart)= 0.00000136 RMS(Int)= 0.00000050

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000050

ITry= 1 IFail=0 DXMaxC= 5.04D-03 DCOld= 1.00D+10 DXMaxT= 7.66D-02 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 4.65D-11 for atom 38.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58086 0.00019 0.00113 -0.00021 0.00093 2.58178

R2 2.73275 -0.00017 -0.00049 0.00006 -0.00044 2.73231

R3 2.58721 -0.00031 -0.00060 -0.00007 -0.00067 2.58655

R4 2.56388 -0.00012 -0.00100 -0.00007 -0.00107 2.56281

R5 3.79471 -0.00025 0.00197 0.00011 0.00207 3.79679

R6 2.77189 0.00021 0.00157 -0.00009 0.00147 2.77336

R7 2.57937 0.00008 0.00039 -0.00005 0.00033 2.57970

R8 2.59806 -0.00003 -0.00023 -0.00000 -0.00024 2.59783

R9 2.81329 0.00002 -0.00009 0.00006 -0.00003 2.81327

R10 2.04300 -0.00001 0.00009 -0.00006 0.00002 2.04302

R11 2.49744 -0.00041 -0.00053 0.00002 -0.00051 2.49693

R12 2.58402 -0.00002 -0.00062 0.00006 -0.00056 2.58346

R13 2.79891 0.00024 0.00104 0.00008 0.00113 2.80004

R14 2.57764 0.00012 0.00037 -0.00007 0.00029 2.57794

R15 3.77674 -0.00019 0.00312 -0.00015 0.00297 3.77971

R16 2.83943 0.00024 0.00107 0.00008 0.00115 2.84058

R17 2.48934 -0.00081 -0.00145 0.00001 -0.00144 2.48790

R18 2.55034 -0.00014 -0.00016 -0.00013 -0.00029 2.55006

R19 2.80755 -0.00014 -0.00045 -0.00006 -0.00051 2.80704

R20 2.04329 -0.00008 -0.00016 0.00005 -0.00011 2.04318

R21 2.48934 -0.00081 -0.00145 0.00001 -0.00144 2.48790

R22 2.55034 -0.00014 -0.00016 -0.00013 -0.00029 2.55006

R23 2.83943 0.00024 0.00107 0.00008 0.00115 2.84058

R24 2.80755 -0.00014 -0.00045 -0.00006 -0.00051 2.80704

R25 2.79891 0.00024 0.00104 0.00008 0.00113 2.80004

R26 2.04329 -0.00008 -0.00016 0.00005 -0.00011 2.04318

R27 2.58402 -0.00002 -0.00062 0.00006 -0.00056 2.58346

R28 2.49744 -0.00041 -0.00053 0.00002 -0.00051 2.49693

R29 2.57764 0.00012 0.00037 -0.00007 0.00029 2.57794

R30 3.77674 -0.00019 0.00312 -0.00015 0.00297 3.77971

R31 2.57937 0.00008 0.00039 -0.00005 0.00033 2.57970

R32 2.56388 -0.00012 -0.00100 -0.00007 -0.00107 2.56281

R33 2.58086 0.00019 0.00113 -0.00021 0.00093 2.58178

R34 3.79471 -0.00025 0.00197 0.00011 0.00207 3.79679

R35 2.77189 0.00021 0.00157 -0.00009 0.00147 2.77336

R36 2.59806 -0.00003 -0.00023 -0.00000 -0.00024 2.59783

R37 2.81329 0.00002 -0.00009 0.00006 -0.00003 2.81327

R38 2.73275 -0.00017 -0.00049 0.00006 -0.00044 2.73231

R39 2.04300 -0.00001 0.00009 -0.00006 0.00002 2.04302

R40 2.58721 -0.00031 -0.00060 -0.00007 -0.00067 2.58655

R41 2.06250 -0.00007 -0.00009 -0.00005 -0.00014 2.06236

R42 2.06991 -0.00015 -0.00027 -0.00014 -0.00041 2.06950

R43 2.06991 -0.00015 -0.00027 -0.00014 -0.00041 2.06950

R44 2.06942 -0.00024 -0.00048 -0.00020 -0.00068 2.06874

R45 2.06942 -0.00024 -0.00048 -0.00020 -0.00068 2.06874

R46 2.06165 -0.00002 -0.00005 -0.00002 -0.00007 2.06158

R47 2.06942 -0.00024 -0.00048 -0.00020 -0.00068 2.06874

R48 2.06942 -0.00024 -0.00048 -0.00020 -0.00068 2.06874

R49 2.06165 -0.00002 -0.00005 -0.00002 -0.00007 2.06158

R50 2.06991 -0.00015 -0.00027 -0.00014 -0.00041 2.06950

R51 2.06991 -0.00015 -0.00027 -0.00014 -0.00041 2.06950

R52 2.06250 -0.00007 -0.00009 -0.00005 -0.00014 2.06236

A1 1.89345 -0.00006 -0.00086 0.00013 -0.00073 1.89271

A2 2.20516 -0.00001 -0.00038 -0.00005 -0.00043 2.20473

A3 2.18458 0.00007 0.00125 -0.00008 0.00117 2.18575

A4 1.90468 0.00028 0.00173 -0.00001 0.00172 1.90640

A5 2.19262 -0.00003 -0.00000 -0.00005 -0.00005 2.19257

A6 2.18589 -0.00024 -0.00173 0.00006 -0.00167 2.18421

A7 1.89749 -0.00040 -0.00185 -0.00003 -0.00188 1.89561

A8 2.22253 0.00012 0.00100 -0.00001 0.00099 2.22353

A9 2.16316 0.00028 0.00085 0.00004 0.00089 2.16405

A10 1.85068 0.00030 0.00100 0.00011 0.00111 1.85179

A11 2.17600 -0.00040 -0.00238 0.00001 -0.00237 2.17363

A12 2.25650 0.00010 0.00137 -0.00012 0.00126 2.25776

A13 1.87847 -0.00011 -0.00002 -0.00020 -0.00021 1.87826

A14 2.18135 -0.00005 -0.00074 0.00022 -0.00052 2.18083

A15 2.22337 0.00016 0.00076 -0.00003 0.00073 2.22410

A16 2.16676 0.00012 0.00119 -0.00002 0.00117 2.16792

A17 2.23157 -0.00014 -0.00033 -0.00004 -0.00037 2.23120

A18 2.16706 0.00012 0.00096 0.00003 0.00099 2.16805

A19 1.88456 0.00002 -0.00063 0.00001 -0.00062 1.88394

A20 1.91302 -0.00015 0.00063 -0.00001 0.00063 1.91365

A21 2.18999 0.00001 -0.00092 0.00009 -0.00083 2.18916

A22 2.18018 0.00015 0.00028 -0.00008 0.00020 2.18038

A23 1.88497 0.00019 -0.00011 -0.00002 -0.00014 1.88483

A24 2.24746 -0.00010 -0.00059 -0.00001 -0.00060 2.24686

A25 2.15076 -0.00008 0.00071 0.00003 0.00074 2.15149

A26 1.85705 -0.00019 -0.00060 0.00006 -0.00054 1.85651

A27 2.15466 0.00004 -0.00039 0.00006 -0.00033 2.15433

A28 2.27148 0.00015 0.00099 -0.00012 0.00087 2.27235

A29 1.88518 0.00014 0.00071 -0.00004 0.00067 1.88585

A30 2.16470 -0.00007 -0.00029 0.00014 -0.00014 2.16456

A31 2.23331 -0.00007 -0.00042 -0.00010 -0.00052 2.23278

A32 2.16900 0.00014 0.00148 0.00011 0.00159 2.17059

A33 1.85705 -0.00019 -0.00060 0.00006 -0.00054 1.85651

A34 2.27148 0.00015 0.00099 -0.00012 0.00087 2.27235

A35 2.15466 0.00004 -0.00039 0.00006 -0.00033 2.15433

A36 1.88518 0.00014 0.00071 -0.00004 0.00067 1.88585

A37 2.23331 -0.00007 -0.00042 -0.00010 -0.00052 2.23278

A38 2.16470 -0.00007 -0.00029 0.00014 -0.00014 2.16456

A39 1.88456 0.00002 -0.00063 0.00001 -0.00062 1.88394

A40 2.16706 0.00012 0.00096 0.00003 0.00099 2.16805

A41 2.23157 -0.00014 -0.00033 -0.00004 -0.00037 2.23120

A42 1.91302 -0.00015 0.00063 -0.00001 0.00063 1.91365

A43 2.18999 0.00001 -0.00092 0.00009 -0.00083 2.18916

A44 2.18018 0.00015 0.00028 -0.00008 0.00020 2.18038

A45 2.15076 -0.00008 0.00071 0.00003 0.00074 2.15149

A46 2.24746 -0.00010 -0.00059 -0.00001 -0.00060 2.24686

A47 1.88497 0.00019 -0.00011 -0.00002 -0.00014 1.88483

A48 2.16676 0.00012 0.00119 -0.00002 0.00117 2.16792

A49 1.90468 0.00028 0.00173 -0.00001 0.00172 1.90640

A50 2.18589 -0.00024 -0.00173 0.00006 -0.00167 2.18421

A51 2.19262 -0.00003 -0.00000 -0.00005 -0.00005 2.19257

A52 2.22253 0.00012 0.00100 -0.00001 0.00099 2.22353

A53 2.16316 0.00028 0.00085 0.00004 0.00089 2.16405

A54 1.89749 -0.00040 -0.00185 -0.00003 -0.00188 1.89561

A55 1.85068 0.00030 0.00100 0.00011 0.00111 1.85179

A56 2.17600 -0.00040 -0.00238 0.00001 -0.00237 2.17363

A57 2.25650 0.00010 0.00137 -0.00012 0.00126 2.25776

A58 1.87847 -0.00011 -0.00002 -0.00020 -0.00021 1.87826

A59 2.22337 0.00016 0.00076 -0.00003 0.00073 2.22410

A60 2.18135 -0.00005 -0.00074 0.00022 -0.00052 2.18083

A61 1.89345 -0.00006 -0.00086 0.00013 -0.00073 1.89271

A62 2.20516 -0.00001 -0.00038 -0.00005 -0.00043 2.20473

A63 2.18458 0.00007 0.00125 -0.00008 0.00117 2.18575

A64 2.16900 0.00014 0.00148 0.00011 0.00159 2.17059

A65 1.56964 0.00014 0.00079 -0.00007 0.00072 1.57035

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A69 1.94257 0.00007 0.00051 0.00006 0.00058 1.94315

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A72 1.88985 -0.00005 -0.00032 -0.00006 -0.00037 1.88947

A73 1.88985 -0.00005 -0.00032 -0.00006 -0.00037 1.88947

A74 1.85761 -0.00001 0.00003 -0.00009 -0.00006 1.85755

A75 1.93438 -0.00012 -0.00059 -0.00005 -0.00064 1.93374

A76 1.93438 -0.00012 -0.00059 -0.00005 -0.00064 1.93374

A77 1.94451 0.00017 0.00079 0.00012 0.00092 1.94542

A78 1.85727 0.00010 0.00048 0.00001 0.00049 1.85776

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D67 2.11253 0.00002 0.00007 0.00003 0.00010 2.11264

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D112 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D115 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

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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

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D125 1.03315 0.00000 0.00004 -0.00001 0.00002 1.03317

D126 -1.03315 -0.00000 -0.00004 0.00001 -0.00002 -1.03317

D127 3.14159 -0.00000 -0.00000 -0.00000 0.00000 3.14159

D128 -2.10844 0.00000 0.00004 -0.00001 0.00002 -2.10842

D129 2.10844 -0.00000 -0.00004 0.00001 -0.00002 2.10842

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D135 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

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Item Value Threshold Converged?

Maximum Force 0.000809 0.000450 NO

RMS Force 0.000135 0.000300 YES

Maximum Displacement 0.005041 0.001800 NO

RMS Displacement 0.001306 0.001200 NO

Predicted change in Energy=-3.599013D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:37:45 2019, MaxMem= 2415919104 cpu: 1.4

(Enter /home/blab/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -2.073173 -2.191589 0.000000

2 7 0 -0.746473 -1.865356 0.000000

3 6 0 -0.006980 -3.002182 0.000000

4 6 0 -0.917489 -4.153190 0.000000

5 6 0 -2.189877 -3.632749 0.000000

6 7 0 1.354196 -3.105846 0.000000

7 6 0 2.177962 -2.072749 0.000000

8 7 0 1.856638 -0.743937 0.000000

9 6 0 2.997646 0.003795 0.000000

10 6 0 4.169627 -0.937469 0.000000

11 6 0 3.655416 -2.185087 0.000000

12 7 0 -3.123780 -1.314277 0.000000

13 6 0 -4.169627 0.937469 0.000000

14 6 0 -3.655416 2.185087 0.000000

15 6 0 -2.177962 2.072749 0.000000

16 7 0 -1.856638 0.743937 0.000000

17 6 0 -2.997646 -0.003795 0.000000

18 7 0 -1.354196 3.105846 0.000000

19 7 0 0.746473 1.865356 0.000000

20 6 0 0.006980 3.002182 0.000000

21 6 0 0.917489 4.153190 0.000000

22 6 0 2.189877 3.632749 0.000000

23 6 0 2.073173 2.191589 0.000000

24 7 0 3.123780 1.314277 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.479397 -5.575988 0.000000

27 1 0 -3.123096 -4.178576 0.000000

28 6 0 5.583966 -0.483465 0.000000

29 1 0 4.190645 -3.124517 0.000000

30 6 0 -5.583966 0.483465 0.000000

31 1 0 -4.190645 3.124517 0.000000

32 6 0 0.479397 5.575988 0.000000

33 1 0 3.123096 4.178576 0.000000

34 1 0 -1.334113 -6.254602 0.000000

35 1 0 0.136821 -5.800314 0.877076

36 1 0 0.136821 -5.800314 -0.877076

37 1 0 5.792710 0.137856 0.876822

38 1 0 5.792710 0.137856 -0.876822

39 1 0 6.274375 -1.328145 0.000000

40 1 0 -5.792710 -0.137856 0.876822

41 1 0 -5.792710 -0.137856 -0.876822

42 1 0 -6.274375 1.328145 0.000000

43 1 0 -0.136821 5.800314 0.877076

44 1 0 -0.136821 5.800314 -0.877076

45 1 0 1.334113 6.254602 0.000000

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Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.366221 0.000000

3 C 2.219508 1.356180 0.000000

4 C 2.276727 2.294217 1.467599 0.000000

5 C 1.445878 2.281906 2.272147 1.374711 0.000000

6 N 3.547213 2.439595 1.365117 2.501496 3.583026

7 C 4.252796 2.931780 2.374409 3.729619 4.638062

8 N 4.187972 2.834390 2.927925 4.395315 4.971873

9 C 5.525660 4.184753 4.250139 5.710413 6.335208

10 C 6.367524 5.002900 4.659087 6.018273 6.907085

11 C 5.728592 4.413485 3.752438 4.978443 6.021891

12 N 1.368742 2.440344 3.544499 3.595435 2.499498

13 C 3.766447 4.424230 5.731359 6.040796 4.980593

14 C 4.653900 4.986786 6.341833 6.904347 5.999586

15 C 4.265625 4.190207 5.519791 6.352253 5.705511

16 N 2.943501 2.835644 4.177876 4.986367 4.389354

17 C 2.375099 2.921163 4.234904 4.641609 3.717768

18 N 5.346003 5.008211 6.254838 7.272161 6.790216

19 N 4.940567 4.018345 4.925507 6.244331 6.233082

20 C 5.594846 4.925507 6.004381 7.214846 6.989170

21 C 7.014292 6.244331 7.214846 8.506651 8.383113

22 C 7.217791 6.233082 6.989170 8.383113 8.483497

23 C 6.033609 4.940567 5.594846 7.014292 7.217791

24 N 6.268925 5.008885 5.332305 6.798901 7.260029

25 Zn 3.016804 2.009173 3.002191 4.253325 4.241748

26 C 3.740893 3.720231 2.616802 1.488717 2.588806

27 H 2.247322 3.316523 3.330778 2.205753 1.081122

28 C 7.845347 6.479512 6.132097 7.465642 8.387528

29 H 6.332912 5.095157 4.199407 5.210682 6.400731

30 C 4.413794 5.377574 6.576664 6.578341 5.335078

31 H 5.722296 6.063098 7.418861 7.979886 7.047249

32 C 8.176238 7.541642 8.591948 9.828948 9.587798

33 H 8.220719 7.176537 7.833305 9.259841 9.446930

34 H 4.129683 4.428408 3.512764 2.142313 2.757978

35 H 4.321601 4.127150 2.935896 2.143327 3.298655

36 H 4.321601 4.127150 2.935896 2.143327 3.298655

37 H 8.250288 6.895114 6.653200 8.013032 8.871752

38 H 8.250288 6.895114 6.653200 8.013032 8.871752

39 H 8.392085 7.041371 6.500602 7.726823 8.772386

40 H 4.338386 5.405329 6.515201 6.376480 5.095439

41 H 4.338386 5.405329 6.515201 6.376480 5.095439

42 H 5.480750 6.384054 7.617872 7.664285 6.426009

43 H 8.269779 7.739731 8.847037 10.022523 9.693657

44 H 8.269779 7.739731 8.847037 10.022523 9.693657

45 H 9.107565 8.382276 9.353426 10.648561 10.496581

6 7 8 9 10

6 N 0.000000

7 C 1.321318 0.000000

8 N 2.414760 1.367111 0.000000

9 C 3.517215 2.232469 1.364186 0.000000

10 C 3.553662 2.292507 2.321071 1.503169 0.000000

11 C 2.478590 1.481718 2.304890 2.285578 1.349431

12 N 4.823069 5.355722 5.012969 6.261723 7.303135

13 C 6.845510 7.025190 6.256436 7.227832 8.547429

14 C 7.286301 7.222013 6.241949 7.001519 8.425061

15 C 6.268492 6.013255 4.920541 5.573822 7.025190

16 N 5.013011 4.920541 4.000274 4.910386 6.256436

17 C 5.344273 5.573822 4.910386 5.995298 7.227832

18 N 6.776467 6.268492 5.013011 5.344273 6.845510

19 N 5.008211 4.190207 2.835644 2.921163 4.424230

20 C 6.254838 5.519791 4.177876 4.234904 5.731359

21 C 7.272161 6.352253 4.986367 4.641609 6.040796

22 C 6.790216 5.705511 4.389354 3.717768 4.980593

23 C 5.346003 4.265625 2.943501 2.375099 3.766447

24 N 4.761188 3.516606 2.417001 1.316538 2.482771

25 Zn 3.388233 3.006627 2.000137 2.997649 4.273715

26 C 3.076307 4.397072 5.367102 6.574482 6.567289

27 H 4.604008 5.704010 6.049339 7.413213 7.980513

28 C 4.976730 3.758548 3.736418 2.631819 1.485421

29 H 2.836511 2.270927 3.333879 3.348072 2.187149

30 C 7.811609 8.172011 7.541161 8.595008 9.856552

31 H 8.340425 8.220142 7.178758 7.836481 9.294831

32 C 8.725796 7.835069 6.468249 6.114811 7.486182

33 H 7.496120 6.322369 5.082819 4.176665 5.221986

34 H 4.140250 5.461004 6.367757 7.611286 7.652650

35 H 3.084060 4.339385 5.412392 6.530029 6.378092

36 H 3.084060 4.339385 5.412392 6.530029 6.378092

37 H 5.566941 4.326892 4.127837 2.932434 2.135308

38 H 5.566941 4.326892 4.127837 2.932434 2.135308

39 H 5.231480 4.163536 4.456198 3.537091 2.140699

40 H 7.788199 8.248893 7.723256 8.835114 10.032764

41 H 7.788199 8.248893 7.723256 8.835114 10.032764

42 H 8.823569 9.110877 8.390882 9.366124 10.686916

43 H 9.072601 8.253037 6.897127 6.647840 8.044407

44 H 9.072601 8.253037 6.897127 6.647840 8.044407

45 H 9.360469 8.369997 7.018018 6.468379 7.730848

11 12 13 14 15

11 C 0.000000

12 N 6.834897 0.000000

13 C 8.425061 2.482771 0.000000

14 C 8.517434 3.539517 1.349431 0.000000

15 C 7.222013 3.516606 2.292507 1.481718 0.000000

16 N 6.241949 2.417001 2.321071 2.304890 1.367111

17 C 7.001519 1.316538 1.503169 2.285578 2.232469

18 N 7.286301 4.761188 3.553662 2.478590 1.321318

19 N 4.986786 5.008885 5.002900 4.413485 2.931780

20 C 6.341833 5.332305 4.659087 3.752438 2.374409

21 C 6.904347 6.798901 6.018273 4.978443 3.729619

22 C 5.999586 7.260029 6.907085 6.021891 4.638062

23 C 4.653900 6.268925 6.367524 5.728592 4.252796

24 N 3.539517 6.778002 7.303135 6.834897 5.355722

25 Zn 4.258717 3.389001 4.273715 4.258717 3.006627

26 C 5.347419 5.015471 7.486182 8.385785 7.835069

27 H 7.065566 2.864300 5.221986 6.385889 6.322369

28 C 2.571930 8.747291 9.856552 9.617034 8.172011

29 H 1.081202 7.535104 9.294831 9.473783 8.220142

30 C 9.617034 3.047029 1.485421 2.571930 3.758548

31 H 9.473783 4.565204 2.187149 1.081202 2.270927

32 C 8.385785 7.775515 6.567289 5.347419 4.397072

33 H 6.385889 8.318347 7.980513 7.065566 5.704010

34 H 6.438661 5.254495 7.730848 8.753102 8.369997

35 H 5.120512 5.614741 8.044407 8.883522 8.253037

36 H 5.120512 5.614741 8.044407 8.883522 8.253037

37 H 3.276112 9.076415 10.032764 9.707062 8.248893

38 H 3.276112 9.076415 10.032764 9.707062 8.248893

39 H 2.755594 9.398166 10.686916 10.532974 9.110877

40 H 9.707062 3.045647 2.135308 3.276112 4.326892

41 H 9.707062 3.045647 2.135308 3.276112 4.326892

42 H 10.532974 4.112011 2.140699 2.755594 4.163536

43 H 8.883522 7.765861 6.378092 5.120512 4.339385

44 H 8.883522 7.765861 6.378092 5.120512 4.339385

45 H 8.753102 8.784118 7.652650 6.438661 5.461004

16 17 18 19 20

16 N 0.000000

17 C 1.364186 0.000000

18 N 2.414760 3.517215 0.000000

19 N 2.834390 4.184753 2.439595 0.000000

20 C 2.927925 4.250139 1.365117 1.356180 0.000000

21 C 4.395315 5.710413 2.501496 2.294217 1.467599

22 C 4.971873 6.335208 3.583026 2.281906 2.272147

23 C 4.187972 5.525660 3.547213 1.366221 2.219508

24 N 5.012969 6.261723 4.823069 2.440344 3.544499

25 Zn 2.000137 2.997649 3.388233 2.009173 3.002191

26 C 6.468249 6.114811 8.725796 7.541642 8.591948

27 H 5.082819 4.176665 7.496120 7.176537 7.833305

28 C 7.541161 8.595008 7.811609 5.377574 6.576664

29 H 7.178758 7.836481 8.340425 6.063098 7.418861

30 C 3.736418 2.631819 4.976730 6.479512 6.132097

31 H 3.333879 3.348072 2.836511 5.095157 4.199407

32 C 5.367102 6.574482 3.076307 3.720231 2.616802

33 H 6.049339 7.413213 4.604008 3.316523 3.330778

34 H 7.018018 6.468379 9.360469 8.382276 9.353426

35 H 6.897127 6.647840 9.072601 7.739731 8.847037

36 H 6.897127 6.647840 9.072601 7.739731 8.847037

37 H 7.723256 8.835114 7.788199 5.405329 6.515201

38 H 7.723256 8.835114 7.788199 5.405329 6.515201

39 H 8.390882 9.366124 8.823569 6.384054 7.617872

40 H 4.127837 2.932434 5.566941 6.895114 6.653200

41 H 4.127837 2.932434 5.566941 6.895114 6.653200

42 H 4.456198 3.537091 5.231480 7.041371 6.500602

43 H 5.412392 6.530029 3.084060 4.127150 2.935896

44 H 5.412392 6.530029 3.084060 4.127150 2.935896

45 H 6.367757 7.611286 4.140250 4.428408 3.512764

21 22 23 24 25

21 C 0.000000

22 C 1.374711 0.000000

23 C 2.276727 1.445878 0.000000

24 N 3.595435 2.499498 1.368742 0.000000

25 Zn 4.253325 4.241748 3.016804 3.389001 0.000000

26 C 9.828948 9.587798 8.176238 7.775515 5.596559

27 H 9.259841 9.446930 8.220719 8.318347 5.216726

28 C 6.578341 5.335078 4.413794 3.047029 5.604856

29 H 7.979886 7.047249 5.722296 4.565204 5.227247

30 C 7.465642 8.387528 7.845347 8.747291 5.604856

31 H 5.210682 6.400731 6.332912 7.535104 5.227247

32 C 1.488717 2.588806 3.740893 5.015471 5.596559

33 H 2.205753 1.081122 2.247322 2.864300 5.216726

34 H 10.648561 10.496581 9.107565 8.784118 6.395303

35 H 10.022523 9.693657 8.269779 7.765861 5.867847

36 H 10.022523 9.693657 8.269779 7.765861 5.867847

37 H 6.376480 5.095439 4.338386 3.045647 5.860317

38 H 6.376480 5.095439 4.338386 3.045647 5.860317

39 H 7.664285 6.426009 5.480750 4.112011 6.413404

40 H 8.013032 8.871752 8.250288 9.076415 5.860317

41 H 8.013032 8.871752 8.250288 9.076415 5.860317

42 H 7.726823 8.772386 8.392085 9.398166 6.413404

43 H 2.143327 3.298655 4.321601 5.614741 5.867847

44 H 2.143327 3.298655 4.321601 5.614741 5.867847

45 H 2.142313 2.757978 4.129683 5.254495 6.395303

26 27 28 29 30

26 C 0.000000

27 H 2.990302 0.000000

28 C 7.918218 9.458688 0.000000

29 H 5.274373 7.389307 2.986051 0.000000

30 C 7.922979 5.271670 11.209713 10.419239 0.000000

31 H 9.458972 7.380707 10.419239 10.454494 2.986051

32 C 11.193117 10.398533 7.922979 9.458972 7.918218

33 H 10.398533 10.433452 5.271670 7.380707 9.458688

34 H 1.091355 2.740500 9.009209 6.349833 7.966353

35 H 1.095130 3.745178 7.662215 4.935853 8.542982

36 H 1.095130 3.745178 7.662215 4.935853 8.542982

37 H 8.529723 9.944446 1.094729 3.738785 11.415648

38 H 8.529723 9.944446 1.094729 3.738785 11.415648

39 H 7.978572 9.820256 1.090939 2.751161 11.995924

40 H 7.653325 4.921694 11.415648 10.457358 1.094729

41 H 7.653325 4.921694 11.415648 10.457358 1.094729

42 H 9.013813 6.344646 11.995924 11.372899 1.090939

43 H 11.415204 10.453007 8.542982 9.957351 7.662215

44 H 11.415204 10.453007 8.542982 9.957351 7.662215

45 H 11.968779 11.345392 7.966353 9.804470 9.009209

31 32 33 34 35

31 H 0.000000

32 C 5.274373 0.000000

33 H 7.389307 2.990302 0.000000

34 H 9.804470 11.968779 11.345392 0.000000

35 H 9.957351 11.415204 10.453007 1.771803 0.000000

36 H 9.957351 11.415204 10.453007 1.771803 1.754152

37 H 10.457358 7.653325 4.921694 9.613738 8.200668

38 H 10.457358 7.653325 4.921694 9.613738 8.386126

39 H 11.372899 9.013813 6.344646 9.064164 7.644549

40 H 3.738785 8.529723 9.944446 7.619873 8.198949

41 H 3.738785 8.529723 9.944446 7.619873 8.384445

42 H 2.751161 7.978572 9.820256 9.050095 9.627441

43 H 4.935853 1.095130 3.745178 12.145936 11.603856

44 H 4.935853 1.095130 3.745178 12.145936 11.735694

45 H 6.349833 1.091355 2.740500 12.790606 12.145936

36 37 38 39 40

36 H 0.000000

37 H 8.386126 0.000000

38 H 8.200668 1.753644 0.000000

39 H 7.644549 1.774818 1.774818 0.000000

40 H 8.384445 11.588700 11.720633 12.157308 0.000000

41 H 8.198949 11.720633 11.588700 12.157308 1.753644

42 H 9.627441 12.157308 12.157308 12.826808 1.774818

43 H 11.735694 8.198949 8.384445 9.627441 8.200668

44 H 11.603856 8.384445 8.198949 9.627441 8.386126

45 H 12.145936 7.619873 7.619873 9.050095 9.613738

41 42 43 44 45

41 H 0.000000

42 H 1.774818 0.000000

43 H 8.386126 7.644549 0.000000

44 H 8.200668 7.644549 1.754152 0.000000

45 H 9.613738 9.064164 1.771803 1.771803 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=0 Diff= 2.23D-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 2.805457 -1.109288 0.000000

2 7 0 2.009172 0.000888 0.000000

3 6 0 2.789389 1.110161 0.000000

4 6 0 4.196476 0.693085 0.000000

5 6 0 4.186629 -0.681590 0.000000

6 7 0 2.379335 2.412237 0.000000

7 6 0 1.113963 2.792650 0.000000

8 7 0 0.000000 2.000137 0.000000

9 6 0 -1.118476 2.781170 0.000000

10 6 0 -0.680652 4.219164 0.000000

11 6 0 0.668714 4.205888 0.000000

12 7 0 2.381853 -2.410831 0.000000

13 6 0 0.680652 -4.219164 0.000000

14 6 0 -0.668714 -4.205888 0.000000

15 6 0 -1.113963 -2.792650 0.000000

16 7 0 -0.000000 -2.000137 0.000000

17 6 0 1.118476 -2.781170 0.000000

18 7 0 -2.379335 -2.412237 0.000000

19 7 0 -2.009172 -0.000888 0.000000

20 6 0 -2.789389 -1.110161 0.000000

21 6 0 -4.196476 -0.693085 0.000000

22 6 0 -4.186629 0.681590 0.000000

23 6 0 -2.805457 1.109288 0.000000

24 7 0 -2.381853 2.410831 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 5.354251 1.628946 0.000000

27 1 0 5.040400 -1.344840 0.000000

28 6 0 -1.628138 5.363169 0.000000

29 1 0 1.341670 5.052132 0.000000

30 6 0 1.628138 -5.363169 0.000000

31 1 0 -1.341670 -5.052132 0.000000

32 6 0 -5.354251 -1.628946 0.000000

33 1 0 -5.040400 1.344840 0.000000

34 1 0 6.302083 1.087956 0.000000

35 1 0 5.333285 2.284391 0.877076

36 1 0 5.333285 2.284391 -0.877076

37 1 0 -2.282523 5.325841 0.876822

38 1 0 -2.282523 5.325841 -0.876822

39 1 0 -1.100852 6.318218 0.000000

40 1 0 2.282523 -5.325841 0.876822

41 1 0 2.282523 -5.325841 -0.876822

42 1 0 1.100852 -6.318218 0.000000

43 1 0 -5.333285 -2.284391 0.877076

44 1 0 -5.333285 -2.284391 -0.877076

45 1 0 -6.302083 -1.087956 0.000000

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Rotational constants (GHZ): 0.1829819 0.1819389 0.0914341

Leave Link 202 at Tue Sep 17 14:37:45 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 101 beta electrons

nuclear repulsion energy 2761.9266810724 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= -0.1142249686 Hartrees.

Nuclear repulsion after empirical dispersion term = 2761.8124561038 Hartrees.

No density basis found on file 724.

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Polarizable Continuum Model (PCM)

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Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 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 = 3494

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.18D-06

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 122

GePol: Fraction of low-weight points (<1% of avg) = 3.49%

GePol: Cavity surface area = 382.046 Ang\*\*2

GePol: Cavity volume = 379.296 Ang\*\*3

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Atomic radii for non-electrostatic terms: SMD-CDS.

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PCM non-electrostatic energy = -0.0107081968 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2761.8017479070 Hartrees.

Leave Link 301 at Tue Sep 17 14:37:46 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= 15327 LenP2D= 41272.

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 14:37:46 2019, MaxMem= 2415919104 cpu: 12.3

(Enter /home/blab/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:37:46 2019, MaxMem= 2415919104 cpu: 1.2

(Enter /home/blab/g09/l401.exe)

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= -0.000000 -0.000000 -0.000000

Rot= 0.996886 0.000000 -0.000000 0.078852 Ang= 9.05 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 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0177 S= 1.0059

Leave Link 401 at Tue Sep 17 14:37:48 2019, MaxMem= 2415919104 cpu: 21.7

(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= 36624108.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.22D-15 for 3486.

Iteration 1 A\*A^-1 deviation from orthogonality is 5.22D-15 for 3135 3061.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.88D-15 for 3486.

Iteration 1 A^-1\*A deviation from orthogonality is 5.74D-12 for 1756 1746.

E= -1275.84266160295

DIIS: error= 1.95D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.84266160295 IErMin= 1 ErrMin= 1.95D-04

ErrMax= 1.95D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.69D-05 BMatP= 3.69D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.95D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.303 Goal= None Shift= 0.000

Gap= 0.393 Goal= None Shift= 0.000

RMSDP=1.09D-05 MaxDP=3.50D-04 OVMax= 1.33D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.08D-05 CP: 1.00D+00

E= -1275.84267169444 Delta-E= -0.000010091484 Rises=F Damp=F

DIIS: error= 5.95D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84267169444 IErMin= 2 ErrMin= 5.95D-05

ErrMax= 5.95D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.38D-06 BMatP= 3.69D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.197D+00 0.803D+00

Coeff: 0.197D+00 0.803D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.83D-06 MaxDP=1.66D-04 DE=-1.01D-05 OVMax= 9.86D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.80D-06 CP: 1.00D+00 9.65D-01

E= -1275.84267093979 Delta-E= 0.000000754651 Rises=F Damp=F

DIIS: error= 8.36D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1275.84267169444 IErMin= 2 ErrMin= 5.95D-05

ErrMax= 8.36D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.20D-05 BMatP= 7.38D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.149D-01 0.568D+00 0.447D+00

Coeff: -0.149D-01 0.568D+00 0.447D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.39D-06 MaxDP=1.00D-04 DE= 7.55D-07 OVMax= 4.39D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.40D-06 CP: 1.00D+00 1.03D+00 5.32D-01

E= -1275.84267345772 Delta-E= -0.000002517938 Rises=F Damp=F

DIIS: error= 1.40D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84267345772 IErMin= 4 ErrMin= 1.40D-05

ErrMax= 1.40D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.67D-07 BMatP= 7.38D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.112D-01 0.221D+00 0.198D+00 0.592D+00

Coeff: -0.112D-01 0.221D+00 0.198D+00 0.592D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=6.55D-07 MaxDP=3.22D-05 DE=-2.52D-06 OVMax= 4.08D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 5.45D-07 CP: 1.00D+00 1.04D+00 6.02D-01 1.15D+00

E= -1275.84267354561 Delta-E= -0.000000087885 Rises=F Damp=F

DIIS: error= 1.14D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84267354561 IErMin= 5 ErrMin= 1.14D-05

ErrMax= 1.14D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.28D-08 BMatP= 1.67D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.228D-02 0.448D-02 0.178D-01 0.321D+00 0.659D+00

Coeff: -0.228D-02 0.448D-02 0.178D-01 0.321D+00 0.659D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=6.09D-07 MaxDP=2.82D-05 DE=-8.79D-08 OVMax= 4.28D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.28D-07 CP: 1.00D+00 1.05D+00 6.51D-01 1.48D+00 1.45D+00

E= -1275.84267360872 Delta-E= -0.000000063109 Rises=F Damp=F

DIIS: error= 1.01D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84267360872 IErMin= 6 ErrMin= 1.01D-05

ErrMax= 1.01D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.66D-08 BMatP= 5.28D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.280D-02-0.572D-01-0.461D-01-0.431D-01 0.776D-01 0.107D+01

Coeff: 0.280D-02-0.572D-01-0.461D-01-0.431D-01 0.776D-01 0.107D+01

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=8.18D-07 MaxDP=4.08D-05 DE=-6.31D-08 OVMax= 6.08D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.65D-07 CP: 1.00D+00 1.07D+00 7.18D-01 1.89D+00 2.28D+00

CP: 1.73D+00

E= -1275.84267366672 Delta-E= -0.000000058006 Rises=F Damp=F

DIIS: error= 6.72D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84267366672 IErMin= 7 ErrMin= 6.72D-06

ErrMax= 6.72D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.85D-08 BMatP= 1.66D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.491D-02-0.639D-01-0.649D-01-0.317D+00-0.604D+00 0.105D+01

Coeff-Com: 0.999D+00

Coeff: 0.491D-02-0.639D-01-0.649D-01-0.317D+00-0.604D+00 0.105D+01

Coeff: 0.999D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.22D-06 MaxDP=5.84D-05 DE=-5.80D-08 OVMax= 9.04D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.87D-07 CP: 1.00D+00 1.08D+00 8.18D-01 2.50D+00 3.00D+00

CP: 3.00D+00 1.72D+00

E= -1275.84267372262 Delta-E= -0.000000055893 Rises=F Damp=F

DIIS: error= 3.96D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84267372262 IErMin= 8 ErrMin= 3.96D-06

ErrMax= 3.96D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.44D-09 BMatP= 1.66D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.974D-03 0.430D-02-0.445D-02-0.104D+00-0.314D+00 0.529D-01

Coeff-Com: 0.422D+00 0.942D+00

Coeff: 0.974D-03 0.430D-02-0.445D-02-0.104D+00-0.314D+00 0.529D-01

Coeff: 0.422D+00 0.942D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=6.35D-07 MaxDP=3.31D-05 DE=-5.59D-08 OVMax= 4.88D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.59D-07 CP: 1.00D+00 1.09D+00 8.67D-01 2.80D+00 3.00D+00

CP: 3.00D+00 2.51D+00 2.32D+00

E= -1275.84267373500 Delta-E= -0.000000012380 Rises=F Damp=F

DIIS: error= 2.20D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84267373500 IErMin= 9 ErrMin= 2.20D-06

ErrMax= 2.20D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.56D-09 BMatP= 3.44D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.109D-02 0.249D-01 0.183D-01 0.413D-01 0.147D-01-0.301D+00

Coeff-Com: -0.826D-01 0.648D+00 0.637D+00

Coeff: -0.109D-02 0.249D-01 0.183D-01 0.413D-01 0.147D-01-0.301D+00

Coeff: -0.826D-01 0.648D+00 0.637D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.13D-07 MaxDP=1.09D-05 DE=-1.24D-08 OVMax= 1.60D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 5.18D-08 CP: 1.00D+00 1.09D+00 8.82D-01 2.89D+00 3.00D+00

CP: 3.00D+00 2.84D+00 2.80D+00 1.15D+00

E= -1275.84267373776 Delta-E= -0.000000002763 Rises=F Damp=F

DIIS: error= 1.07D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84267373776 IErMin=10 ErrMin= 1.07D-06

ErrMax= 1.07D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.85D-10 BMatP= 2.56D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.549D-03 0.472D-02 0.475D-02 0.450D-01 0.125D+00-0.109D+00

Coeff-Com: -0.201D+00-0.628D-01 0.123D+00 0.107D+01

Coeff: -0.549D-03 0.472D-02 0.475D-02 0.450D-01 0.125D+00-0.109D+00

Coeff: -0.201D+00-0.628D-01 0.123D+00 0.107D+01

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.53D-07 MaxDP=8.46D-06 DE=-2.76D-09 OVMax= 1.18D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 6.10D-08 CP: 1.00D+00 1.10D+00 8.91D-01 2.95D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.37D+00 1.54D+00

E= -1275.84267373887 Delta-E= -0.000000001107 Rises=F Damp=F

DIIS: error= 8.45D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84267373887 IErMin=11 ErrMin= 8.45D-07

ErrMax= 8.45D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.62D-10 BMatP= 3.85D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.135D-03-0.301D-02-0.122D-02 0.233D-01 0.885D-01 0.157D-01

Coeff-Com: -0.138D+00-0.238D+00-0.164D+00 0.791D+00 0.625D+00

Coeff: -0.135D-03-0.301D-02-0.122D-02 0.233D-01 0.885D-01 0.157D-01

Coeff: -0.138D+00-0.238D+00-0.164D+00 0.791D+00 0.625D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=7.96D-08 MaxDP=4.08D-06 DE=-1.11D-09 OVMax= 5.83D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 3.32D-08 CP: 1.00D+00 1.10D+00 8.96D-01 2.98D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.42D+00 2.04D+00

CP: 1.78D+00

E= -1275.84267373924 Delta-E= -0.000000000371 Rises=F Damp=F

DIIS: error= 3.36D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84267373924 IErMin=12 ErrMin= 3.36D-07

ErrMax= 3.36D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.15D-11 BMatP= 3.62D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.139D-03-0.345D-02-0.250D-02-0.405D-02-0.570D-02 0.537D-01

Coeff-Com: -0.664D-02-0.711D-01-0.143D+00 0.254D-01 0.225D+00 0.932D+00

Coeff: 0.139D-03-0.345D-02-0.250D-02-0.405D-02-0.570D-02 0.537D-01

Coeff: -0.664D-02-0.711D-01-0.143D+00 0.254D-01 0.225D+00 0.932D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=5.06D-08 MaxDP=2.71D-06 DE=-3.71D-10 OVMax= 3.87D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 9.79D-09 CP: 1.00D+00 1.10D+00 8.99D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.48D+00 2.31D+00

CP: 2.31D+00 1.37D+00

E= -1275.84267373939 Delta-E= -0.000000000154 Rises=F Damp=F

DIIS: error= 1.77D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84267373939 IErMin=13 ErrMin= 1.77D-07

ErrMax= 1.77D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.13D-11 BMatP= 5.15D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.143D-03-0.185D-02-0.159D-02-0.918D-02-0.286D-01 0.318D-01

Coeff-Com: 0.258D-01 0.197D-01-0.528D-01-0.189D+00-0.331D-01 0.622D+00

Coeff-Com: 0.617D+00

Coeff: 0.143D-03-0.185D-02-0.159D-02-0.918D-02-0.286D-01 0.318D-01

Coeff: 0.258D-01 0.197D-01-0.528D-01-0.189D+00-0.331D-01 0.622D+00

Coeff: 0.617D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.47D-08 MaxDP=1.77D-06 DE=-1.54D-10 OVMax= 2.65D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 2.18D-08 CP: 1.00D+00 1.10D+00 9.02D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.53D+00 2.43D+00

CP: 2.60D+00 1.76D+00 1.36D+00

E= -1275.84267373941 Delta-E= -0.000000000023 Rises=F Damp=F

DIIS: error= 4.19D-08 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84267373941 IErMin=14 ErrMin= 4.19D-08

ErrMax= 4.19D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.26D-12 BMatP= 3.13D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.423D-05 0.563D-03 0.361D-03-0.139D-02-0.805D-02-0.424D-02

Coeff-Com: 0.700D-02 0.318D-01 0.234D-01-0.831D-01-0.750D-01-0.118D-01

Coeff-Com: 0.207D+00 0.913D+00

Coeff: 0.423D-05 0.563D-03 0.361D-03-0.139D-02-0.805D-02-0.424D-02

Coeff: 0.700D-02 0.318D-01 0.234D-01-0.831D-01-0.750D-01-0.118D-01

Coeff: 0.207D+00 0.913D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.07D-08 MaxDP=5.35D-07 DE=-2.32D-11 OVMax= 8.00D-06

Cycle 15 Pass 1 IDiag 1:

RMSU= 2.19D-09 CP: 1.00D+00 1.10D+00 9.03D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.54D+00 2.46D+00

CP: 2.69D+00 1.85D+00 1.61D+00 1.31D+00

E= -1275.84267373938 Delta-E= 0.000000000030 Rises=F Damp=F

DIIS: error= 2.25D-08 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=14 EnMin= -1275.84267373941 IErMin=15 ErrMin= 2.25D-08

ErrMax= 2.25D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.51D-13 BMatP= 2.26D-12

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.123D-04 0.490D-03 0.338D-03 0.169D-04-0.129D-02-0.616D-02

Coeff-Com: 0.128D-02 0.144D-01 0.191D-01-0.231D-01-0.323D-01-0.802D-01

Coeff-Com: 0.267D-01 0.436D+00 0.644D+00

Coeff: -0.123D-04 0.490D-03 0.338D-03 0.169D-04-0.129D-02-0.616D-02

Coeff: 0.128D-02 0.144D-01 0.191D-01-0.231D-01-0.323D-01-0.802D-01

Coeff: 0.267D-01 0.436D+00 0.644D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.66D-09 MaxDP=1.76D-07 DE= 3.05D-11 OVMax= 2.66D-06

Error on total polarization charges = 0.06464

SCF Done: E(UB3LYP) = -1275.84267374 A.U. after 15 cycles

NFock= 15 Conv=0.37D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0178 S= 1.0059

<L.S>= 0.000000000000E+00

KE= 1.320807900382D+03 PE=-8.575564325767D+03 EE= 3.217112003738D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.72

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0178, after 2.0002

Leave Link 502 at Tue Sep 17 14:39:05 2019, MaxMem= 2415919104 cpu: 1357.5

(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= 15327 LenP2D= 41272.

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 = 244

Leave Link 701 at Tue Sep 17 14:39:09 2019, MaxMem= 2415919104 cpu: 68.0

(Enter /home/blab/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Tue Sep 17 14:39:09 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 14:39:19 2019, MaxMem= 2415919104 cpu: 177.5

(Enter /home/blab/g09/l716.exe)

Dipole = 2.75335310D-13-5.28466160D-14 0.00000000D+00

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000005752 0.000022093 0.000000000

2 7 -0.000240949 -0.000753946 -0.000000000

3 6 0.000035083 0.000049492 0.000000000

4 6 -0.000057109 0.000012981 -0.000000000

5 6 0.000014019 0.000023082 -0.000000000

6 7 -0.000074836 -0.000038675 0.000000000

7 6 0.000014159 0.000033717 -0.000000000

8 7 0.000760995 -0.000334514 -0.000000000

9 6 0.000003591 0.000059531 0.000000000

10 6 0.000050178 -0.000051110 0.000000000

11 6 -0.000020352 0.000029406 0.000000000

12 7 0.000033488 0.000019382 -0.000000000

13 6 -0.000050178 0.000051110 0.000000000

14 6 0.000020352 -0.000029406 0.000000000

15 6 -0.000014159 -0.000033717 -0.000000000

16 7 -0.000760995 0.000334514 0.000000000

17 6 -0.000003591 -0.000059531 0.000000000

18 7 0.000074836 0.000038675 0.000000000

19 7 0.000240949 0.000753946 0.000000000

20 6 -0.000035083 -0.000049492 -0.000000000

21 6 0.000057109 -0.000012981 0.000000000

22 6 -0.000014019 -0.000023082 -0.000000000

23 6 -0.000005752 -0.000022093 0.000000000

24 7 -0.000033488 -0.000019382 -0.000000000

25 30 0.000000000 0.000000000 0.000000000

26 6 0.000040951 0.000023330 -0.000000000

27 1 -0.000006314 -0.000019275 0.000000000

28 6 -0.000051959 0.000016510 -0.000000000

29 1 0.000032428 -0.000011016 -0.000000000

30 6 0.000051959 -0.000016510 -0.000000000

31 1 -0.000032428 0.000011016 -0.000000000

32 6 -0.000040951 -0.000023330 -0.000000000

33 1 0.000006314 0.000019275 0.000000000

34 1 -0.000015883 0.000017380 0.000000000

35 1 0.000010382 -0.000009233 0.000005313

36 1 0.000010382 -0.000009233 -0.000005313

37 1 0.000017138 0.000004445 0.000001630

38 1 0.000017138 0.000004445 -0.000001630

39 1 -0.000019021 -0.000014169 -0.000000000

40 1 -0.000017138 -0.000004445 0.000001630

41 1 -0.000017138 -0.000004445 -0.000001630

42 1 0.000019021 0.000014169 -0.000000000

43 1 -0.000010382 0.000009233 0.000005313

44 1 -0.000010382 0.000009233 -0.000005313

45 1 0.000015883 -0.000017380 0.000000000

-------------------------------------------------------------------

Cartesian Forces: Max 0.000760995 RMS 0.000141669

Leave Link 716 at Tue Sep 17 14:39:19 2019, MaxMem= 2415919104 cpu: 0.4

(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 0.000580693 RMS 0.000077723

Search for a local minimum.

Step number 29 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 12 13 14 15

16 17 18 19 20

21 22 23 24 25

26 27 28 29

DE= 8.79D-05 DEPred=-3.60D-06 R=-2.44D+01

Trust test=-2.44D+01 RLast= 1.10D-02 DXMaxT set to 5.00D-02

ITU= -1 1 1 -1 1 -1 -1 1 0 0 1 -1 -1 1 1 -1 1 1 1 -1

ITU= 0 1 -1 1 1 1 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01336

Eigenvalues --- 0.01338 0.01346 0.01347 0.01604 0.01623

Eigenvalues --- 0.01631 0.01640 0.01774 0.01793 0.01809

Eigenvalues --- 0.01823 0.01890 0.01909 0.01939 0.01950

Eigenvalues --- 0.01997 0.02000 0.02045 0.02047 0.02070

Eigenvalues --- 0.02087 0.02103 0.02110 0.02115 0.02205

Eigenvalues --- 0.02301 0.02312 0.02316 0.02351 0.02372

Eigenvalues --- 0.06727 0.07195 0.07195 0.07197 0.07197

Eigenvalues --- 0.07253 0.07314 0.07393 0.08472 0.11407

Eigenvalues --- 0.13586 0.13717 0.14498 0.14500 0.15391

Eigenvalues --- 0.15788 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16022 0.16336 0.16910 0.18776

Eigenvalues --- 0.19503 0.20897 0.22059 0.22091 0.23179

Eigenvalues --- 0.23841 0.23854 0.24371 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25156

Eigenvalues --- 0.25535 0.27237 0.28353 0.30454 0.32394

Eigenvalues --- 0.32817 0.33189 0.33197 0.33282 0.33282

Eigenvalues --- 0.33675 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33724 0.33769 0.34193 0.34402

Eigenvalues --- 0.34437 0.34437 0.34515 0.35555 0.35564

Eigenvalues --- 0.35610 0.35682 0.35682 0.35743 0.36033

Eigenvalues --- 0.38487 0.40519 0.41637 0.41816 0.45623

Eigenvalues --- 0.46392 0.48965 0.48980 0.49854 0.51358

Eigenvalues --- 0.51361 0.52149 0.53239 0.54020 0.54026

Eigenvalues --- 0.54898 0.56320 0.56328 1.98036

Cosine: 0.495 < 0.840

Cut down GDIIS temporarily because of the cosine check. E 7

DIIS coeff's: 2.19206 -1.19206

Cosine: 1.000 > 0.970

Length: 1.000

GDIIS step was calculated using 2 of the last 29 vectors.

Iteration 1 RMS(Cart)= 0.00444508 RMS(Int)= 0.00000607

Iteration 2 RMS(Cart)= 0.00001352 RMS(Int)= 0.00000165

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000165

ITry= 1 IFail=0 DXMaxC= 1.61D-02 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 2.09D-09 for atom 27.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58178 -0.00003 0.00110 0.00164 0.00275 2.58454

R2 2.73231 0.00001 -0.00052 -0.00096 -0.00148 2.73083

R3 2.58655 0.00014 -0.00079 -0.00024 -0.00103 2.58552

R4 2.56281 -0.00008 -0.00127 -0.00283 -0.00409 2.55871

R5 3.79679 0.00049 0.00247 0.00659 0.00906 3.80585

R6 2.77336 -0.00001 0.00175 0.00244 0.00420 2.77756

R7 2.57970 0.00010 0.00040 0.00125 0.00164 2.58134

R8 2.59783 0.00005 -0.00028 -0.00028 -0.00057 2.59726

R9 2.81327 -0.00001 -0.00003 -0.00007 -0.00010 2.81317

R10 2.04302 0.00002 0.00003 -0.00011 -0.00008 2.04294

R11 2.49693 0.00017 -0.00061 -0.00004 -0.00064 2.49629

R12 2.58346 -0.00005 -0.00067 -0.00183 -0.00250 2.58096

R13 2.80004 0.00003 0.00134 0.00269 0.00404 2.80408

R14 2.57794 -0.00003 0.00035 0.00066 0.00101 2.57895

R15 3.77971 0.00058 0.00354 0.00890 0.01243 3.79214

R16 2.84058 0.00005 0.00137 0.00269 0.00407 2.84464

R17 2.48790 0.00011 -0.00172 -0.00224 -0.00396 2.48394

R18 2.55006 0.00005 -0.00034 -0.00070 -0.00104 2.54902

R19 2.80704 -0.00003 -0.00061 -0.00144 -0.00205 2.80499

R20 2.04318 0.00003 -0.00013 -0.00004 -0.00017 2.04301

R21 2.48790 0.00011 -0.00172 -0.00224 -0.00396 2.48394

R22 2.55006 0.00005 -0.00034 -0.00070 -0.00104 2.54902

R23 2.84058 0.00005 0.00137 0.00269 0.00407 2.84464

R24 2.80704 -0.00003 -0.00061 -0.00144 -0.00205 2.80499

R25 2.80004 0.00003 0.00134 0.00269 0.00404 2.80408

R26 2.04318 0.00003 -0.00013 -0.00004 -0.00017 2.04301

R27 2.58346 -0.00005 -0.00067 -0.00183 -0.00250 2.58096

R28 2.49693 0.00017 -0.00061 -0.00004 -0.00064 2.49629

R29 2.57794 -0.00003 0.00035 0.00066 0.00101 2.57895

R30 3.77971 0.00058 0.00354 0.00890 0.01243 3.79214

R31 2.57970 0.00010 0.00040 0.00125 0.00164 2.58134

R32 2.56281 -0.00008 -0.00127 -0.00283 -0.00409 2.55871

R33 2.58178 -0.00003 0.00110 0.00164 0.00275 2.58454

R34 3.79679 0.00049 0.00247 0.00659 0.00906 3.80585

R35 2.77336 -0.00001 0.00175 0.00244 0.00420 2.77756

R36 2.59783 0.00005 -0.00028 -0.00028 -0.00057 2.59726

R37 2.81327 -0.00001 -0.00003 -0.00007 -0.00010 2.81317

R38 2.73231 0.00001 -0.00052 -0.00096 -0.00148 2.73083

R39 2.04302 0.00002 0.00003 -0.00011 -0.00008 2.04294

R40 2.58655 0.00014 -0.00079 -0.00024 -0.00103 2.58552

R41 2.06236 0.00000 -0.00016 -0.00030 -0.00046 2.06190

R42 2.06950 0.00001 -0.00049 -0.00082 -0.00131 2.06818

R43 2.06950 0.00001 -0.00049 -0.00082 -0.00131 2.06818

R44 2.06874 0.00001 -0.00081 -0.00135 -0.00217 2.06657

R45 2.06874 0.00001 -0.00081 -0.00135 -0.00217 2.06657

R46 2.06158 -0.00000 -0.00008 -0.00025 -0.00033 2.06125

R47 2.06874 0.00001 -0.00081 -0.00135 -0.00217 2.06657

R48 2.06874 0.00001 -0.00081 -0.00135 -0.00217 2.06657

R49 2.06158 -0.00000 -0.00008 -0.00025 -0.00033 2.06125

R50 2.06950 0.00001 -0.00049 -0.00082 -0.00131 2.06818

R51 2.06950 0.00001 -0.00049 -0.00082 -0.00131 2.06818

R52 2.06236 0.00000 -0.00016 -0.00030 -0.00046 2.06190

A1 1.89271 -0.00009 -0.00088 -0.00212 -0.00299 1.88972

A2 2.20473 0.00003 -0.00052 -0.00040 -0.00091 2.20381

A3 2.18575 0.00007 0.00139 0.00251 0.00390 2.18965

A4 1.90640 0.00016 0.00205 0.00433 0.00639 1.91279

A5 2.19257 -0.00009 -0.00006 -0.00077 -0.00083 2.19174

A6 2.18421 -0.00006 -0.00199 -0.00356 -0.00556 2.17866

A7 1.89561 -0.00009 -0.00224 -0.00422 -0.00647 1.88914

A8 2.22353 0.00004 0.00118 0.00242 0.00360 2.22713

A9 2.16405 0.00005 0.00106 0.00180 0.00286 2.16691

A10 1.85179 0.00003 0.00132 0.00244 0.00376 1.85555

A11 2.17363 -0.00005 -0.00282 -0.00469 -0.00752 2.16612

A12 2.25776 0.00002 0.00150 0.00226 0.00376 2.26152

A13 1.87826 0.00000 -0.00026 -0.00043 -0.00069 1.87757

A14 2.18083 0.00001 -0.00061 -0.00070 -0.00131 2.17952

A15 2.22410 -0.00001 0.00087 0.00113 0.00200 2.22610

A16 2.16792 0.00011 0.00139 0.00245 0.00384 2.17177

A17 2.23120 -0.00001 -0.00044 -0.00060 -0.00104 2.23015

A18 2.16805 0.00010 0.00118 0.00229 0.00347 2.17152

A19 1.88394 -0.00009 -0.00074 -0.00169 -0.00243 1.88152

A20 1.91365 0.00016 0.00075 0.00213 0.00288 1.91653

A21 2.18916 -0.00007 -0.00099 -0.00183 -0.00283 2.18633

A22 2.18038 -0.00008 0.00024 -0.00030 -0.00005 2.18033

A23 1.88483 -0.00010 -0.00016 -0.00095 -0.00111 1.88372

A24 2.24686 -0.00001 -0.00072 -0.00090 -0.00162 2.24524

A25 2.15149 0.00011 0.00088 0.00185 0.00273 2.15422

A26 1.85651 0.00002 -0.00064 -0.00093 -0.00158 1.85493

A27 2.15433 0.00001 -0.00039 -0.00027 -0.00066 2.15367

A28 2.27235 -0.00002 0.00103 0.00120 0.00223 2.27458

A29 1.88585 0.00002 0.00080 0.00144 0.00223 1.88808

A30 2.16456 0.00001 -0.00017 0.00006 -0.00011 2.16445

A31 2.23278 -0.00003 -0.00062 -0.00150 -0.00212 2.23066

A32 2.17059 0.00014 0.00190 0.00349 0.00539 2.17599

A33 1.85651 0.00002 -0.00064 -0.00093 -0.00158 1.85493

A34 2.27235 -0.00002 0.00103 0.00120 0.00223 2.27458

A35 2.15433 0.00001 -0.00039 -0.00027 -0.00066 2.15367

A36 1.88585 0.00002 0.00080 0.00144 0.00223 1.88808

A37 2.23278 -0.00003 -0.00062 -0.00150 -0.00212 2.23066

A38 2.16456 0.00001 -0.00017 0.00006 -0.00011 2.16445

A39 1.88394 -0.00009 -0.00074 -0.00169 -0.00243 1.88152

A40 2.16805 0.00010 0.00118 0.00229 0.00347 2.17152

A41 2.23120 -0.00001 -0.00044 -0.00060 -0.00104 2.23015

A42 1.91365 0.00016 0.00075 0.00213 0.00288 1.91653

A43 2.18916 -0.00007 -0.00099 -0.00183 -0.00283 2.18633

A44 2.18038 -0.00008 0.00024 -0.00030 -0.00005 2.18033

A45 2.15149 0.00011 0.00088 0.00185 0.00273 2.15422

A46 2.24686 -0.00001 -0.00072 -0.00090 -0.00162 2.24524

A47 1.88483 -0.00010 -0.00016 -0.00095 -0.00111 1.88372

A48 2.16792 0.00011 0.00139 0.00245 0.00384 2.17177

A49 1.90640 0.00016 0.00205 0.00433 0.00639 1.91279

A50 2.18421 -0.00006 -0.00199 -0.00356 -0.00556 2.17866

A51 2.19257 -0.00009 -0.00006 -0.00077 -0.00083 2.19174

A52 2.22353 0.00004 0.00118 0.00242 0.00360 2.22713

A53 2.16405 0.00005 0.00106 0.00180 0.00286 2.16691

A54 1.89561 -0.00009 -0.00224 -0.00422 -0.00647 1.88914

A55 1.85179 0.00003 0.00132 0.00244 0.00376 1.85555

A56 2.17363 -0.00005 -0.00282 -0.00469 -0.00752 2.16612

A57 2.25776 0.00002 0.00150 0.00226 0.00376 2.26152

A58 1.87826 0.00000 -0.00026 -0.00043 -0.00069 1.87757

A59 2.22410 -0.00001 0.00087 0.00113 0.00200 2.22610

A60 2.18083 0.00001 -0.00061 -0.00070 -0.00131 2.17952

A61 1.89271 -0.00009 -0.00088 -0.00212 -0.00299 1.88972

A62 2.20473 0.00003 -0.00052 -0.00040 -0.00091 2.20381

A63 2.18575 0.00007 0.00139 0.00251 0.00390 2.18965

A64 2.17059 0.00014 0.00190 0.00349 0.00539 2.17599

A65 1.57035 -0.00001 0.00085 0.00113 0.00198 1.57233

A66 1.57124 0.00001 -0.00085 -0.00113 -0.00198 1.56926

A67 1.57124 0.00001 -0.00085 -0.00113 -0.00198 1.56926

A68 1.57035 -0.00001 0.00085 0.00113 0.00198 1.57233

A69 1.94315 -0.00004 0.00069 0.00065 0.00134 1.94449

A70 1.94052 0.00002 0.00010 0.00038 0.00048 1.94100

A71 1.94052 0.00002 0.00010 0.00038 0.00048 1.94100

A72 1.88947 0.00001 -0.00044 -0.00056 -0.00101 1.88846

A73 1.88947 0.00001 -0.00044 -0.00056 -0.00101 1.88846

A74 1.85755 -0.00001 -0.00007 -0.00037 -0.00044 1.85711

A75 1.93374 0.00003 -0.00076 -0.00091 -0.00168 1.93206

A76 1.93374 0.00003 -0.00076 -0.00091 -0.00168 1.93206

A77 1.94542 -0.00005 0.00110 0.00110 0.00219 1.94762

A78 1.85776 -0.00001 0.00058 0.00067 0.00125 1.85900

A79 1.89523 0.00000 -0.00008 0.00003 -0.00004 1.89518

A80 1.89523 0.00000 -0.00008 0.00003 -0.00004 1.89518

A81 1.93374 0.00003 -0.00076 -0.00091 -0.00168 1.93206

A82 1.93374 0.00003 -0.00076 -0.00091 -0.00168 1.93206

A83 1.94542 -0.00005 0.00110 0.00110 0.00219 1.94762

A84 1.85776 -0.00001 0.00058 0.00067 0.00125 1.85900

A85 1.89523 0.00000 -0.00008 0.00003 -0.00004 1.89518

A86 1.89523 0.00000 -0.00008 0.00003 -0.00004 1.89518

A87 1.94052 0.00002 0.00010 0.00038 0.00048 1.94100

A88 1.94052 0.00002 0.00010 0.00038 0.00048 1.94100

A89 1.94315 -0.00004 0.00069 0.00065 0.00134 1.94449

A90 1.85755 -0.00001 -0.00007 -0.00037 -0.00044 1.85711

A91 1.88947 0.00001 -0.00044 -0.00056 -0.00101 1.88846

A92 1.88947 0.00001 -0.00044 -0.00056 -0.00101 1.88846

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

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D125 1.03317 0.00000 0.00002 0.00001 0.00004 1.03321

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D127 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D128 -2.10842 0.00000 0.00002 0.00001 0.00004 -2.10838

D129 2.10842 -0.00000 -0.00002 -0.00001 -0.00004 2.10838

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 0.000581 0.000450 NO

RMS Force 0.000078 0.000300 YES

Maximum Displacement 0.016130 0.001800 NO

RMS Displacement 0.004448 0.001200 NO

Predicted change in Energy=-1.758586D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:39:19 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

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1 6 0 -2.079681 -2.192406 0.000000

2 7 0 -0.750846 -1.868769 0.000000

3 6 0 -0.007805 -3.000689 0.000000

4 6 0 -0.922336 -4.151343 0.000000

5 6 0 -2.195205 -3.632876 0.000000

6 7 0 1.354298 -3.103645 0.000000

7 6 0 2.181231 -2.073518 0.000000

8 7 0 1.863184 -0.745279 0.000000

9 6 0 3.004156 0.003485 0.000000

10 6 0 4.177378 -0.939669 0.000000

11 6 0 3.660836 -2.185730 0.000000

12 7 0 -3.127123 -1.312163 0.000000

13 6 0 -4.177378 0.939669 0.000000

14 6 0 -3.660836 2.185730 0.000000

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24 7 0 3.127123 1.312163 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.476838 -5.571785 0.000000

27 1 0 -3.128679 -4.178178 0.000000

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29 1 0 4.196101 -3.125037 0.000000

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32 6 0 0.476838 5.571785 0.000000

33 1 0 3.128679 4.178178 0.000000

34 1 0 -1.326895 -6.255839 0.000000

35 1 0 0.140174 -5.793261 0.876376

36 1 0 0.140174 -5.793261 -0.876376

37 1 0 5.797187 0.135022 0.876312

38 1 0 5.797187 0.135022 -0.876312

39 1 0 6.282911 -1.328610 0.000000

40 1 0 -5.797187 -0.135022 0.876312

41 1 0 -5.797187 -0.135022 -0.876312

42 1 0 -6.282911 1.328610 0.000000

43 1 0 -0.140174 5.793261 0.876376

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45 1 0 1.326895 6.255839 0.000000

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Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.367677 0.000000

3 C 2.223958 1.354014 0.000000

4 C 2.275275 2.289007 1.469820 0.000000

5 C 1.445094 2.279966 2.276923 1.374410 0.000000

6 N 3.552824 2.440604 1.365988 2.506139 3.588740

7 C 4.262570 2.939218 2.377294 3.734901 4.645944

8 N 4.200042 2.845239 2.930439 4.400044 4.980837

9 C 5.537809 4.195876 4.254053 5.716637 6.344799

10 C 6.381233 5.015040 4.665143 6.026768 6.918322

11 C 5.740521 4.423054 3.758070 4.986894 6.032201

12 N 1.368197 2.440594 3.547008 3.594722 2.500836

13 C 3.769646 4.430400 5.736877 6.042657 4.983691

14 C 4.654904 4.990692 6.343782 6.903468 6.000354

15 C 4.267133 4.193761 5.520087 6.350883 5.706411

16 N 2.945652 2.840870 4.180276 4.986191 4.390726

17 C 2.376138 2.925182 4.238083 4.640980 3.718451

18 N 5.345497 5.008897 6.251074 7.267836 6.788802

19 N 4.950255 4.027936 4.928202 6.248303 6.240778

20 C 5.596948 4.928202 6.001398 7.212262 6.989809

21 C 7.018209 6.248303 7.212262 8.505140 8.385292

22 C 7.225549 6.240778 6.989809 8.385292 8.489219

23 C 6.043746 4.950255 5.596948 7.018209 7.225549

24 N 6.276369 5.015673 5.331835 6.800589 7.265024

25 Zn 3.021873 2.013968 3.000699 4.252570 4.244610

26 C 3.740228 3.713140 2.613528 1.488666 2.590783

27 H 2.245816 3.314734 3.335616 2.206506 1.081078

28 C 7.857857 6.490509 6.137358 7.473625 8.397814

29 H 6.344701 5.103969 4.205745 5.220316 6.411450

30 C 4.415754 5.382080 6.581990 6.579893 5.337743

31 H 5.723149 6.066949 7.420670 7.978924 7.047905

32 C 8.174256 7.541158 8.586163 9.823284 9.584654

33 H 8.228691 7.184448 7.834135 9.262378 9.452846

34 H 4.132574 4.424728 3.512264 2.143029 2.762951

35 H 4.319947 4.118688 2.930596 2.143096 3.299893

36 H 4.319947 4.118688 2.930596 2.143096 3.299893

37 H 8.260138 6.903610 6.655714 8.018281 8.879375

38 H 8.260138 6.903610 6.655714 8.018281 8.879375

39 H 8.407085 7.054468 6.509144 7.738437 8.785675

40 H 4.338272 5.407342 6.518965 6.376748 5.096780

41 H 4.338272 5.407342 6.518965 6.376748 5.096780

42 H 5.483129 6.389599 7.623633 7.665876 6.428506

43 H 8.264418 7.736127 8.838502 10.013738 9.687272

44 H 8.264418 7.736127 8.838502 10.013738 9.687272

45 H 9.109204 8.386076 9.352258 10.647463 10.497231

6 7 8 9 10

6 N 0.000000

7 C 1.320977 0.000000

8 N 2.412645 1.365787 0.000000

9 C 3.517995 2.234087 1.364722 0.000000

10 C 3.557046 2.295695 2.322344 1.505321 0.000000

11 C 2.482477 1.483854 2.303574 2.285583 1.348882

12 N 4.826234 5.362675 5.022402 6.270846 7.313993

13 C 6.851848 7.036420 6.271159 7.242297 8.563519

14 C 7.288968 7.229865 6.253448 7.013153 8.438349

15 C 6.269209 6.019052 4.929798 5.583303 7.036420

16 N 5.016612 4.929798 4.013425 4.923541 6.271159

17 C 5.348561 5.583303 4.923541 6.008315 7.242297

18 N 6.772513 6.269209 5.016612 5.348561 6.851848

19 N 5.008897 4.193761 2.840870 2.925182 4.430400

20 C 6.251074 5.520087 4.180276 4.238083 5.736877

21 C 7.267836 6.350883 4.986191 4.640980 6.042657

22 C 6.788802 5.706411 4.390726 3.718451 4.983691

23 C 5.345497 4.267133 2.945652 2.376138 3.769646

24 N 4.758389 3.515330 2.414666 1.314442 2.484710

25 Zn 3.386256 3.009526 2.006712 3.004158 4.281760

26 C 3.073235 4.393542 5.363848 6.572744 6.566447

27 H 4.609957 5.711807 6.058341 7.422801 7.991646

28 C 4.979935 3.760966 3.736438 2.632298 1.484336

29 H 2.841884 2.272750 3.332529 3.347892 2.185448

30 C 7.817613 8.182358 7.554746 8.608269 9.871425

31 H 8.342865 8.227718 7.189873 7.847788 9.307899

32 C 8.719692 7.832983 6.467400 6.115006 7.489529

33 H 7.494890 6.323082 5.083494 4.176550 5.224187

34 H 4.138251 5.458824 6.367329 7.611645 7.652365

35 H 3.078338 4.332486 5.405453 6.524775 6.373727

36 H 3.078338 4.332486 5.405453 6.524775 6.373727

37 H 5.567419 4.326743 4.125437 2.930230 2.132291

38 H 5.567419 4.326743 4.125437 2.930230 2.132291

39 H 5.238509 4.168772 4.458056 3.539027 2.141155

40 H 7.792584 8.257169 7.734443 8.845944 10.045263

41 H 7.792584 8.257169 7.734443 8.845944 10.045263

42 H 8.830166 9.122291 8.405943 9.381128 10.703399

43 H 9.064018 8.248829 6.894489 6.646529 8.046219

44 H 9.064018 8.248829 6.894489 6.646529 8.046219

45 H 9.359524 8.373057 7.021628 6.473417 7.739547

11 12 13 14 15

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12 N 6.843940 0.000000

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17 C 7.013153 1.314442 1.505321 2.285583 2.234087

18 N 7.288968 4.758389 3.557046 2.482477 1.320977

19 N 4.990692 5.015673 5.015040 4.423054 2.939218

20 C 6.343782 5.331835 4.665143 3.758070 2.377294

21 C 6.903468 6.800589 6.026768 4.986894 3.734901

22 C 6.000354 7.265024 6.918322 6.032201 4.645944

23 C 4.654904 6.276369 6.381233 5.740521 4.262570

24 N 3.538376 6.782527 7.313993 6.843940 5.362675

25 Zn 4.263700 3.391264 4.281760 4.263700 3.009526

26 C 5.346562 5.016811 7.489529 8.385516 7.832983

27 H 7.075830 2.866016 5.224187 6.386119 6.323082

28 C 2.571771 8.756804 9.871425 9.629415 8.182358

29 H 1.081113 7.544277 9.307899 9.483444 8.227718

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32 C 8.385516 7.770282 6.566447 5.346562 4.393542

33 H 6.386119 8.323395 7.991646 7.075830 5.711807

34 H 6.437644 5.261250 7.739547 8.758274 8.373057

35 H 5.116383 5.614580 8.046219 8.881442 8.248829

36 H 5.116383 5.614580 8.046219 8.881442 8.248829

37 H 3.273806 9.083258 10.045263 9.717382 8.257169

38 H 3.273806 9.083258 10.045263 9.717382 8.257169

39 H 2.758610 9.410048 10.703399 10.546502 9.122291

40 H 9.717382 3.046772 2.132291 3.273806 4.326743

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42 H 10.546502 4.114934 2.141155 2.758610 4.168772

43 H 8.881442 7.757380 6.373727 5.116383 4.332486

44 H 8.881442 7.757380 6.373727 5.116383 4.332486

45 H 8.758274 8.781397 7.652365 6.437644 5.458824

16 17 18 19 20

16 N 0.000000

17 C 1.364722 0.000000

18 N 2.412645 3.517995 0.000000

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20 C 2.930439 4.254053 1.365988 1.354014 0.000000

21 C 4.400044 5.716637 2.506139 2.289007 1.469820

22 C 4.980837 6.344799 3.588740 2.279966 2.276923

23 C 4.200042 5.537809 3.552824 1.367677 2.223958

24 N 5.022402 6.270846 4.826234 2.440594 3.547008

25 Zn 2.006712 3.004158 3.386256 2.013968 3.000699

26 C 6.467400 6.115006 8.719692 7.541158 8.586163

27 H 5.083494 4.176550 7.494890 7.184448 7.834135

28 C 7.554746 8.608269 7.817613 5.382080 6.581990

29 H 7.189873 7.847788 8.342865 6.066949 7.420670

30 C 3.736438 2.632298 4.979935 6.490509 6.137358

31 H 3.332529 3.347892 2.841884 5.103969 4.205745

32 C 5.363848 6.572744 3.073235 3.713140 2.613528

33 H 6.058341 7.422801 4.609957 3.314734 3.335616

34 H 7.021628 6.473417 9.359524 8.386076 9.352258

35 H 6.894489 6.646529 9.064018 7.736127 8.838502

36 H 6.894489 6.646529 9.064018 7.736127 8.838502

37 H 7.734443 8.845944 7.792584 5.407342 6.518965

38 H 7.734443 8.845944 7.792584 5.407342 6.518965

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40 H 4.125437 2.930230 5.567419 6.903610 6.655714

41 H 4.125437 2.930230 5.567419 6.903610 6.655714

42 H 4.458056 3.539027 5.238509 7.054468 6.509144

43 H 5.405453 6.524775 3.078338 4.118688 2.930596

44 H 5.405453 6.524775 3.078338 4.118688 2.930596

45 H 6.367329 7.611645 4.138251 4.424728 3.512264

21 22 23 24 25

21 C 0.000000

22 C 1.374410 0.000000

23 C 2.275275 1.445094 0.000000

24 N 3.594722 2.500836 1.368197 0.000000

25 Zn 4.252570 4.244610 3.021873 3.391264 0.000000

26 C 9.823284 9.584654 8.174256 7.770282 5.592152

27 H 9.262378 9.452846 8.228691 8.323395 5.219752

28 C 6.579893 5.337743 4.415754 3.049767 5.611656

29 H 7.978924 7.047905 5.723149 4.564149 5.231933

30 C 7.473625 8.397814 7.857857 8.756804 5.611656

31 H 5.220316 6.411450 6.344701 7.544277 5.231933

32 C 1.488666 2.590783 3.740228 5.016811 5.592152

33 H 2.206506 1.081078 2.245816 2.866016 5.219752

34 H 10.647463 10.497231 9.109204 8.781397 6.395011

35 H 10.013738 9.687272 8.264418 7.757380 5.860850

36 H 10.013738 9.687272 8.264418 7.757380 5.860850

37 H 6.376748 5.096780 4.338272 3.046772 5.864599

38 H 6.376748 5.096780 4.338272 3.046772 5.864599

39 H 7.665876 6.428506 5.483129 4.114934 6.421851

40 H 8.018281 8.879375 8.260138 9.083258 5.864599

41 H 8.018281 8.879375 8.260138 9.083258 5.864599

42 H 7.738437 8.785675 8.407085 9.410048 6.421851

43 H 2.143096 3.299893 4.319947 5.614580 5.860850

44 H 2.143096 3.299893 4.319947 5.614580 5.860850

45 H 2.143029 2.762951 4.132574 5.261250 6.395011

26 27 28 29 30

26 C 0.000000

27 H 2.995731 0.000000

28 C 7.917185 9.468897 0.000000

29 H 5.274745 7.400102 2.985065 0.000000

30 C 7.927413 5.273801 11.223312 10.431538 0.000000

31 H 9.458733 7.380809 10.431538 10.463865 2.985065

32 C 11.184305 10.395265 7.927413 9.458733 7.917185

33 H 10.395265 10.439503 5.273801 7.380809 9.468897

34 H 1.091113 2.750109 9.008105 6.348654 7.976700

35 H 1.094436 3.749924 7.658011 4.933355 8.546072

36 H 1.094436 3.749924 7.658011 4.933355 8.546072

37 H 8.526369 9.952020 1.093583 3.736226 11.426832

38 H 8.526369 9.952020 1.093583 3.736226 11.426832

39 H 7.981149 9.833517 1.090764 2.753529 12.011326

40 H 7.657181 4.923004 11.426832 10.467755 1.093583

41 H 7.657181 4.923004 11.426832 10.467755 1.093583

42 H 9.018090 6.346172 12.011326 11.386161 1.090764

43 H 11.403756 10.446473 8.546072 9.955268 7.658011

44 H 11.403756 10.446473 8.546072 9.955268 7.658011

45 H 11.964370 11.345521 7.976700 9.809851 9.008105

31 32 33 34 35

31 H 0.000000

32 C 5.274745 0.000000

33 H 7.400102 2.995731 0.000000

34 H 9.809851 11.964370 11.345521 0.000000

35 H 9.955268 11.403756 10.446473 1.770397 0.000000

36 H 9.955268 11.403756 10.446473 1.770397 1.752752

37 H 10.467755 7.657181 4.923004 9.610597 8.194286

38 H 10.467755 7.657181 4.923004 9.610597 8.379633

39 H 11.386161 9.018090 6.346172 9.065690 7.644237

40 H 3.736226 8.526369 9.952020 7.629929 8.201702

41 H 3.736226 8.526369 9.952020 7.629929 8.386885

42 H 2.753529 7.981149 9.833517 9.060130 9.630426

43 H 4.933355 1.094436 3.749924 12.139075 11.589913

44 H 4.933355 1.094436 3.749924 12.139075 11.721699

45 H 6.348654 1.091113 2.750109 12.790023 12.139075

36 37 38 39 40

36 H 0.000000

37 H 8.379633 0.000000

38 H 8.194286 1.752624 0.000000

39 H 7.644237 1.773717 1.773717 0.000000

40 H 8.386885 11.597517 11.729199 12.170511 0.000000

41 H 8.201702 11.729199 11.597517 12.170511 1.752624

42 H 9.630426 12.170511 12.170511 12.843703 1.773717

43 H 11.721699 8.201702 8.386885 9.630426 8.194286

44 H 11.589913 8.386885 8.201702 9.630426 8.379633

45 H 12.139075 7.629929 7.629929 9.060130 9.610597

41 42 43 44 45

41 H 0.000000

42 H 1.773717 0.000000

43 H 8.379633 7.644237 0.000000

44 H 8.194286 7.644237 1.752752 0.000000

45 H 9.610597 9.065690 1.770397 1.770397 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=0 Diff= 8.38D-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 2.807975 -1.116688 0.000000

2 7 0 2.013966 -0.003095 0.000000

3 6 0 2.788965 1.107188 0.000000

4 6 0 4.196970 0.685413 0.000000

5 6 0 4.188321 -0.688970 0.000000

6 7 0 2.378682 2.410105 0.000000

7 6 0 1.115117 2.795311 0.000000

8 7 0 0.000000 2.006712 0.000000

9 6 0 -1.118959 2.787991 0.000000

10 6 0 -0.678989 4.227581 0.000000

11 6 0 0.669788 4.210763 0.000000

12 7 0 2.379703 -2.416130 0.000000

13 6 0 0.678989 -4.227581 0.000000

14 6 0 -0.669788 -4.210763 0.000000

15 6 0 -1.115117 -2.795311 0.000000

16 7 0 -0.000000 -2.006712 0.000000

17 6 0 1.118959 -2.787991 0.000000

18 7 0 -2.378682 -2.410105 0.000000

19 7 0 -2.013966 0.003095 0.000000

20 6 0 -2.788965 -1.107188 0.000000

21 6 0 -4.196970 -0.685413 0.000000

22 6 0 -4.188321 0.688970 0.000000

23 6 0 -2.807975 1.116688 0.000000

24 7 0 -2.379703 2.416130 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 5.350362 1.626590 0.000000

27 1 0 5.041307 -1.353156 0.000000

28 6 0 -1.625330 5.371125 0.000000

29 1 0 1.343118 5.056595 0.000000

30 6 0 1.625330 -5.371125 0.000000

31 1 0 -1.343118 -5.056595 0.000000

32 6 0 -5.350362 -1.626590 0.000000

33 1 0 -5.041307 1.353156 0.000000

34 1 0 6.301194 1.091385 0.000000

35 1 0 5.326842 2.281726 0.876376

36 1 0 5.326842 2.281726 -0.876376

37 1 0 -2.278400 5.332401 0.876312

38 1 0 -2.278400 5.332401 -0.876312

39 1 0 -1.099847 6.326967 0.000000

40 1 0 2.278400 -5.332401 0.876312

41 1 0 2.278400 -5.332401 -0.876312

42 1 0 1.099847 -6.326967 0.000000

43 1 0 -5.326842 -2.281726 0.876376

44 1 0 -5.326842 -2.281726 -0.876376

45 1 0 -6.301194 -1.091385 0.000000

---------------------------------------------------------------------

Rotational constants (GHZ): 0.1830657 0.1813867 0.0913150

Leave Link 202 at Tue Sep 17 14:39:19 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 101 beta electrons

nuclear repulsion energy 2760.3802927079 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= -0.1142262310 Hartrees.

Nuclear repulsion after empirical dispersion term = 2760.2660664769 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 = 3498

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.41D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 134

GePol: Fraction of low-weight points (<1% of avg) = 3.83%

GePol: Cavity surface area = 382.349 Ang\*\*2

GePol: Cavity volume = 379.545 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0107534611 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2760.2553130158 Hartrees.

Leave Link 301 at Tue Sep 17 14:39:19 2019, MaxMem= 2415919104 cpu: 1.9

(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= 41252.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.86D-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 14:39:20 2019, MaxMem= 2415919104 cpu: 13.0

(Enter /home/blab/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:39:20 2019, MaxMem= 2415919104 cpu: 1.5

(Enter /home/blab/g09/l401.exe)

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= -0.000000 -0.000000 -0.000000

Rot= 1.000000 -0.000000 -0.000000 0.000386 Ang= 0.04 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 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0178 S= 1.0059

Leave Link 401 at Tue Sep 17 14:39:21 2019, MaxMem= 2415919104 cpu: 21.9

(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= 36708012.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.88D-15 for 3490.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.80D-15 for 2020 1850.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.88D-15 for 3490.

Iteration 1 A^-1\*A deviation from orthogonality is 1.98D-12 for 1758 1748.

E= -1275.84245547494

DIIS: error= 6.53D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.84245547494 IErMin= 1 ErrMin= 6.53D-04

ErrMax= 6.53D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.36D-04 BMatP= 4.36D-04

IDIUse=3 WtCom= 9.93D-01 WtEn= 6.53D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.303 Goal= None Shift= 0.000

Gap= 0.393 Goal= None Shift= 0.000

RMSDP=3.04D-05 MaxDP=8.76D-04 OVMax= 4.65D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.04D-05 CP: 1.00D+00

E= -1275.84255922822 Delta-E= -0.000103753286 Rises=F Damp=F

DIIS: error= 2.09D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84255922822 IErMin= 2 ErrMin= 2.09D-04

ErrMax= 2.09D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.01D-05 BMatP= 4.36D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.09D-03

Coeff-Com: 0.142D+00 0.858D+00

Coeff-En: 0.000D+00 0.100D+01

Coeff: 0.142D+00 0.858D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.19D-05 MaxDP=5.02D-04 DE=-1.04D-04 OVMax= 3.44D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.18D-05 CP: 1.00D+00 9.80D-01

E= -1275.84255010565 Delta-E= 0.000009122575 Rises=F Damp=F

DIIS: error= 2.51D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1275.84255922822 IErMin= 2 ErrMin= 2.09D-04

ErrMax= 2.51D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.16D-04 BMatP= 6.01D-05

IDIUse=3 WtCom= 3.87D-01 WtEn= 6.13D-01

Coeff-Com: -0.119D-01 0.589D+00 0.423D+00

Coeff-En: 0.000D+00 0.608D+00 0.392D+00

Coeff: -0.459D-02 0.601D+00 0.404D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=6.99D-06 MaxDP=3.00D-04 DE= 9.12D-06 OVMax= 1.26D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 4.03D-06 CP: 1.00D+00 1.04D+00 5.48D-01

E= -1275.84257417937 Delta-E= -0.000024073722 Rises=F Damp=F

DIIS: error= 5.23D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84257417937 IErMin= 4 ErrMin= 5.23D-05

ErrMax= 5.23D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.35D-06 BMatP= 6.01D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.942D-02 0.220D+00 0.160D+00 0.629D+00

Coeff: -0.942D-02 0.220D+00 0.160D+00 0.629D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.15D-06 MaxDP=1.07D-04 DE=-2.41D-05 OVMax= 1.41D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.57D-06 CP: 1.00D+00 1.06D+00 6.13D-01 1.29D+00

E= -1275.84257509317 Delta-E= -0.000000913797 Rises=F Damp=F

DIIS: error= 3.84D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84257509317 IErMin= 5 ErrMin= 3.84D-05

ErrMax= 3.84D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.58D-07 BMatP= 1.35D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.183D-02 0.130D-02 0.338D-02 0.333D+00 0.664D+00

Coeff: -0.183D-02 0.130D-02 0.338D-02 0.333D+00 0.664D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.04D-06 MaxDP=9.36D-05 DE=-9.14D-07 OVMax= 1.43D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 6.65D-07 CP: 1.00D+00 1.07D+00 6.71D-01 1.70D+00 1.38D+00

E= -1275.84257579274 Delta-E= -0.000000699570 Rises=F Damp=F

DIIS: error= 3.35D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84257579274 IErMin= 6 ErrMin= 3.35D-05

ErrMax= 3.35D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.84D-07 BMatP= 5.58D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.322D-02-0.755D-01-0.534D-01-0.103D+00 0.737D-01 0.116D+01

Coeff: 0.322D-02-0.755D-01-0.534D-01-0.103D+00 0.737D-01 0.116D+01

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.05D-06 MaxDP=1.49D-04 DE=-7.00D-07 OVMax= 2.25D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.60D-07 CP: 1.00D+00 1.09D+00 7.65D-01 2.26D+00 2.28D+00

CP: 1.85D+00

E= -1275.84257650090 Delta-E= -0.000000708163 Rises=F Damp=F

DIIS: error= 2.15D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84257650090 IErMin= 7 ErrMin= 2.15D-05

ErrMax= 2.15D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.98D-07 BMatP= 1.84D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.435D-02-0.718D-01-0.543D-01-0.352D+00-0.537D+00 0.108D+01

Coeff-Com: 0.927D+00

Coeff: 0.435D-02-0.718D-01-0.543D-01-0.352D+00-0.537D+00 0.108D+01

Coeff: 0.927D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.82D-06 MaxDP=1.82D-04 DE=-7.08D-07 OVMax= 2.81D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 6.86D-07 CP: 1.00D+00 1.12D+00 8.81D-01 2.97D+00 3.00D+00

CP: 3.00D+00 1.61D+00

E= -1275.84257704526 Delta-E= -0.000000544359 Rises=F Damp=F

DIIS: error= 1.20D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84257704526 IErMin= 8 ErrMin= 1.20D-05

ErrMax= 1.20D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.60D-08 BMatP= 1.84D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.481D-03 0.104D-01 0.247D-02-0.859D-01-0.269D+00 0.142D-01

Coeff-Com: 0.394D+00 0.933D+00

Coeff: 0.481D-03 0.104D-01 0.247D-02-0.859D-01-0.269D+00 0.142D-01

Coeff: 0.394D+00 0.933D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.83D-06 MaxDP=9.53D-05 DE=-5.44D-07 OVMax= 1.41D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.29D-06 CP: 1.00D+00 1.13D+00 9.32D-01 3.00D+00 3.00D+00

CP: 3.00D+00 2.31D+00 2.29D+00

E= -1275.84257715537 Delta-E= -0.000000110116 Rises=F Damp=F

DIIS: error= 6.94D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84257715537 IErMin= 9 ErrMin= 6.94D-06

ErrMax= 6.94D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.50D-08 BMatP= 3.60D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.111D-02 0.302D-01 0.177D-01 0.576D-01 0.144D-01-0.324D+00

Coeff-Com: -0.563D-01 0.625D+00 0.636D+00

Coeff: -0.111D-02 0.302D-01 0.177D-01 0.576D-01 0.144D-01-0.324D+00

Coeff: -0.563D-01 0.625D+00 0.636D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=5.94D-07 MaxDP=3.08D-05 DE=-1.10D-07 OVMax= 4.44D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.66D-07 CP: 1.00D+00 1.13D+00 9.46D-01 3.00D+00 3.00D+00

CP: 3.00D+00 2.58D+00 2.80D+00 1.29D+00

E= -1275.84257718073 Delta-E= -0.000000025354 Rises=F Damp=F

DIIS: error= 3.31D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84257718073 IErMin=10 ErrMin= 3.31D-06

ErrMax= 3.31D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.11D-09 BMatP= 2.50D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.476D-03 0.584D-02 0.314D-02 0.466D-01 0.110D+00-0.127D+00

Coeff-Com: -0.179D+00-0.295D-01 0.157D+00 0.101D+01

Coeff: -0.476D-03 0.584D-02 0.314D-02 0.466D-01 0.110D+00-0.127D+00

Coeff: -0.179D+00-0.295D-01 0.157D+00 0.101D+01

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.53D-07 MaxDP=2.53D-05 DE=-2.54D-08 OVMax= 3.46D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.77D-07 CP: 1.00D+00 1.13D+00 9.57D-01 3.00D+00 3.00D+00

CP: 3.00D+00 2.85D+00 3.00D+00 1.50D+00 1.33D+00

E= -1275.84257719141 Delta-E= -0.000000010684 Rises=F Damp=F

DIIS: error= 2.55D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84257719141 IErMin=11 ErrMin= 2.55D-06

ErrMax= 2.55D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.29D-09 BMatP= 4.11D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.755D-05-0.548D-02-0.338D-02 0.162D-01 0.744D-01 0.242D-01

Coeff-Com: -0.122D+00-0.222D+00-0.174D+00 0.717D+00 0.695D+00

Coeff: -0.755D-05-0.548D-02-0.338D-02 0.162D-01 0.744D-01 0.242D-01

Coeff: -0.122D+00-0.222D+00-0.174D+00 0.717D+00 0.695D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.56D-07 MaxDP=1.34D-05 DE=-1.07D-08 OVMax= 1.86D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 9.08D-08 CP: 1.00D+00 1.13D+00 9.63D-01 3.00D+00 3.00D+00

CP: 3.00D+00 2.98D+00 3.00D+00 1.62D+00 1.84D+00

CP: 1.75D+00

E= -1275.84257719530 Delta-E= -0.000000003891 Rises=F Damp=F

DIIS: error= 1.02D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84257719530 IErMin=12 ErrMin= 1.02D-06

ErrMax= 1.02D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.01D-10 BMatP= 3.29D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.148D-03-0.498D-02-0.291D-02-0.490D-02 0.371D-02 0.576D-01

Coeff-Com: -0.222D-01-0.951D-01-0.160D+00 0.104D+00 0.323D+00 0.802D+00

Coeff: 0.148D-03-0.498D-02-0.291D-02-0.490D-02 0.371D-02 0.576D-01

Coeff: -0.222D-01-0.951D-01-0.160D+00 0.104D+00 0.323D+00 0.802D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.45D-07 MaxDP=7.81D-06 DE=-3.89D-09 OVMax= 1.10D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 3.72D-08 CP: 1.00D+00 1.13D+00 9.66D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.69D+00 2.05D+00

CP: 2.20D+00 1.26D+00

E= -1275.84257719630 Delta-E= -0.000000000996 Rises=F Damp=F

DIIS: error= 5.72D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84257719630 IErMin=13 ErrMin= 5.72D-07

ErrMax= 5.72D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.74D-10 BMatP= 6.01D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.977D-04-0.134D-02-0.731D-03-0.811D-02-0.233D-01 0.263D-01

Coeff-Com: 0.180D-01 0.218D-01-0.425D-01-0.164D+00-0.458D-01 0.497D+00

Coeff-Com: 0.723D+00

Coeff: 0.977D-04-0.134D-02-0.731D-03-0.811D-02-0.233D-01 0.263D-01

Coeff: 0.180D-01 0.218D-01-0.425D-01-0.164D+00-0.458D-01 0.497D+00

Coeff: 0.723D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.15D-07 MaxDP=5.75D-06 DE=-9.96D-10 OVMax= 8.69D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 2.43D-08 CP: 1.00D+00 1.13D+00 9.69D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.75D+00 2.18D+00

CP: 2.48D+00 1.62D+00 1.48D+00

E= -1275.84257719663 Delta-E= -0.000000000329 Rises=F Damp=F

DIIS: error= 1.68D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84257719663 IErMin=14 ErrMin= 1.68D-07

ErrMax= 1.68D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.96D-11 BMatP= 2.74D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.917D-05 0.765D-03 0.476D-03-0.225D-02-0.124D-01-0.157D-02

Coeff-Com: 0.124D-01 0.398D-01 0.204D-01-0.118D+00-0.105D+00 0.713D-01

Coeff-Com: 0.377D+00 0.717D+00

Coeff: 0.917D-05 0.765D-03 0.476D-03-0.225D-02-0.124D-01-0.157D-02

Coeff: 0.124D-01 0.398D-01 0.204D-01-0.118D+00-0.105D+00 0.713D-01

Coeff: 0.377D+00 0.717D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.43D-08 MaxDP=1.25D-06 DE=-3.29D-10 OVMax= 1.76D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 7.37D-09 CP: 1.00D+00 1.13D+00 9.70D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.77D+00 2.21D+00

CP: 2.55D+00 1.67D+00 1.64D+00 1.13D+00

E= -1275.84257719667 Delta-E= -0.000000000043 Rises=F Damp=F

DIIS: error= 7.76D-08 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.84257719667 IErMin=15 ErrMin= 7.76D-08

ErrMax= 7.76D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.26D-12 BMatP= 3.96D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.114D-04 0.543D-03 0.308D-03 0.288D-04-0.183D-02-0.538D-02

Coeff-Com: 0.295D-02 0.136D-01 0.170D-01-0.281D-01-0.344D-01-0.549D-01

Coeff-Com: 0.367D-01 0.293D+00 0.761D+00

Coeff: -0.114D-04 0.543D-03 0.308D-03 0.288D-04-0.183D-02-0.538D-02

Coeff: 0.295D-02 0.136D-01 0.170D-01-0.281D-01-0.344D-01-0.549D-01

Coeff: 0.367D-01 0.293D+00 0.761D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.33D-08 MaxDP=6.68D-07 DE=-4.32D-11 OVMax= 9.72D-06

Cycle 16 Pass 1 IDiag 1:

RMSU= 2.40D-09 CP: 1.00D+00 1.13D+00 9.70D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.77D+00 2.22D+00

CP: 2.58D+00 1.71D+00 1.73D+00 1.22D+00 1.01D+00

E= -1275.84257719666 Delta-E= 0.000000000010 Rises=F Damp=F

DIIS: error= 3.34D-08 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=15 EnMin= -1275.84257719667 IErMin=16 ErrMin= 3.34D-08

ErrMax= 3.34D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.40D-12 BMatP= 5.26D-12

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.598D-05 0.115D-03 0.558D-04 0.408D-03 0.134D-02-0.201D-02

Coeff-Com: -0.470D-03-0.736D-03 0.462D-02 0.507D-02 0.119D-02-0.353D-01

Coeff-Com: -0.308D-01 0.305D-01 0.375D+00 0.651D+00

Coeff: -0.598D-05 0.115D-03 0.558D-04 0.408D-03 0.134D-02-0.201D-02

Coeff: -0.470D-03-0.736D-03 0.462D-02 0.507D-02 0.119D-02-0.353D-01

Coeff: -0.308D-01 0.305D-01 0.375D+00 0.651D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.29D-09 MaxDP=2.17D-07 DE= 1.05D-11 OVMax= 3.18D-06

Error on total polarization charges = 0.06464

SCF Done: E(UB3LYP) = -1275.84257720 A.U. after 16 cycles

NFock= 16 Conv=0.43D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0180 S= 1.0060

<L.S>= 0.000000000000E+00

KE= 1.320804520485D+03 PE=-8.572457025258D+03 EE= 3.215554614561D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.75

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0180, after 2.0002

Leave Link 502 at Tue Sep 17 14:40:44 2019, MaxMem= 2415919104 cpu: 1454.5

(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= 15325 LenP2D= 41252.

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 = 246

Leave Link 701 at Tue Sep 17 14:40:48 2019, MaxMem= 2415919104 cpu: 71.8

(Enter /home/blab/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Tue Sep 17 14:40:48 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 14:40:58 2019, MaxMem= 2415919104 cpu: 176.9

(Enter /home/blab/g09/l716.exe)

Dipole =-1.84741111D-13-8.97060204D-14-1.11022302D-15

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.001477329 -0.000027779 -0.000000000

2 7 0.000867977 0.002660792 0.000000000

3 6 -0.001885099 -0.000258150 0.000000000

4 6 0.001887397 -0.001078680 -0.000000000

5 6 -0.000149586 0.000216595 0.000000000

6 7 -0.000600694 -0.001163637 0.000000000

7 6 0.000739971 0.001167542 0.000000000

8 7 -0.000848369 0.000212111 0.000000000

9 6 -0.000099884 -0.001894113 -0.000000000

10 6 -0.001761697 0.000598228 -0.000000000

11 6 -0.000487797 -0.000947205 0.000000000

12 7 -0.000871054 -0.001833548 -0.000000000

13 6 0.001761697 -0.000598228 -0.000000000

14 6 0.000487797 0.000947205 -0.000000000

15 6 -0.000739971 -0.001167542 0.000000000

16 7 0.000848369 -0.000212111 0.000000000

17 6 0.000099884 0.001894113 0.000000000

18 7 0.000600694 0.001163637 -0.000000000

19 7 -0.000867977 -0.002660792 0.000000000

20 6 0.001885099 0.000258150 -0.000000000

21 6 -0.001887397 0.001078680 0.000000000

22 6 0.000149586 -0.000216595 0.000000000

23 6 -0.001477329 0.000027779 0.000000000

24 7 0.000871054 0.001833548 -0.000000000

25 30 -0.000000000 -0.000000000 -0.000000000

26 6 -0.000896842 -0.000174155 0.000000000

27 1 0.000111272 -0.000252669 0.000000000

28 6 -0.000000275 -0.000445835 0.000000000

29 1 0.000016965 -0.000166636 0.000000000

30 6 0.000000275 0.000445835 -0.000000000

31 1 -0.000016965 0.000166636 0.000000000

32 6 0.000896842 0.000174155 0.000000000

33 1 -0.000111272 0.000252669 -0.000000000

34 1 -0.000231584 -0.000080699 0.000000000

35 1 0.000276527 0.000016731 0.000393521

36 1 0.000276527 0.000016731 -0.000393521

37 1 0.000298948 0.000488141 0.000520062

38 1 0.000298948 0.000488141 -0.000520062

39 1 -0.000052710 -0.000193848 0.000000000

40 1 -0.000298948 -0.000488141 0.000520062

41 1 -0.000298948 -0.000488141 -0.000520062

42 1 0.000052710 0.000193848 0.000000000

43 1 -0.000276527 -0.000016731 0.000393521

44 1 -0.000276527 -0.000016731 -0.000393521

45 1 0.000231584 0.000080699 -0.000000000

-------------------------------------------------------------------

Cartesian Forces: Max 0.002660792 RMS 0.000750651

Leave Link 716 at Tue Sep 17 14:40:58 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 0.001752895 RMS 0.000405176

Search for a local minimum.

Step number 30 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 12 13 14 15

16 17 18 19 20

21 22 23 24 25

26 27 28 29 30

DE= 9.65D-05 DEPred=-1.76D-05 R=-5.49D+00

Trust test=-5.49D+00 RLast= 3.86D-02 DXMaxT set to 5.00D-02

ITU= -1 -1 1 1 -1 1 -1 -1 1 0 0 1 -1 -1 1 1 -1 1 1 1

ITU= -1 0 1 -1 1 1 1 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01340

Eigenvalues --- 0.01342 0.01346 0.01347 0.01604 0.01623

Eigenvalues --- 0.01631 0.01640 0.01775 0.01793 0.01810

Eigenvalues --- 0.01822 0.01890 0.01909 0.01940 0.01949

Eigenvalues --- 0.01998 0.02000 0.02045 0.02048 0.02070

Eigenvalues --- 0.02088 0.02103 0.02111 0.02115 0.02206

Eigenvalues --- 0.02313 0.02317 0.02351 0.02373 0.04782

Eigenvalues --- 0.07184 0.07184 0.07187 0.07190 0.07190

Eigenvalues --- 0.07307 0.07409 0.07423 0.11820 0.13354

Eigenvalues --- 0.14453 0.14496 0.14498 0.15178 0.15378

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16014 0.16154 0.16565 0.16726 0.18963

Eigenvalues --- 0.21235 0.22067 0.22102 0.22342 0.23097

Eigenvalues --- 0.23840 0.23853 0.24379 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25119

Eigenvalues --- 0.25405 0.27509 0.28238 0.32065 0.32317

Eigenvalues --- 0.33194 0.33200 0.33250 0.33282 0.33282

Eigenvalues --- 0.33723 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33724 0.33833 0.34382 0.34437

Eigenvalues --- 0.34437 0.34478 0.34684 0.35554 0.35563

Eigenvalues --- 0.35639 0.35682 0.35682 0.35757 0.37612

Eigenvalues --- 0.38367 0.40675 0.41638 0.41830 0.42734

Eigenvalues --- 0.46589 0.48970 0.48992 0.49225 0.51127

Eigenvalues --- 0.51356 0.51362 0.52912 0.53923 0.54015

Eigenvalues --- 0.54019 0.56324 0.56333 0.56511

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 0.06100 0.40481 0.08267 0.17536 0.04471

DIIS coeff's: 0.00018 -0.01898 0.00689 0.02276 0.03206

DIIS coeff's: 0.00412 0.03245 -0.00308 0.30605 -0.10082

DIIS coeff's: -0.09174 0.02658 -0.00422 0.01160 0.00762

Cosine: 0.998 > 0.000

Length: 1.083

GDIIS step was calculated using 20 of the last 30 vectors.

Iteration 1 RMS(Cart)= 0.00427031 RMS(Int)= 0.00000570

Iteration 2 RMS(Cart)= 0.00001279 RMS(Int)= 0.00000024

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000024

ITry= 1 IFail=0 DXMaxC= 1.55D-02 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 3.47D-10 for atom 33.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58454 -0.00062 -0.00284 -0.00001 -0.00285 2.58169

R2 2.73083 0.00057 0.00156 0.00000 0.00156 2.73239

R3 2.58552 0.00021 0.00113 -0.00000 0.00113 2.58665

R4 2.55871 0.00056 0.00385 0.00000 0.00385 2.56256

R5 3.80585 -0.00079 -0.00800 0.00001 -0.00799 3.79786

R6 2.77756 -0.00036 -0.00406 0.00001 -0.00405 2.77350

R7 2.58134 -0.00071 -0.00156 0.00000 -0.00156 2.57978

R8 2.59726 -0.00005 0.00060 0.00001 0.00060 2.59786

R9 2.81317 0.00004 0.00010 0.00000 0.00011 2.81328

R10 2.04294 0.00003 0.00010 -0.00000 0.00010 2.04304

R11 2.49629 0.00057 0.00082 0.00001 0.00083 2.49711

R12 2.58096 0.00013 0.00224 0.00000 0.00225 2.58321

R13 2.80408 -0.00084 -0.00388 -0.00000 -0.00388 2.80020

R14 2.57895 -0.00029 -0.00109 0.00000 -0.00108 2.57787

R15 3.79214 -0.00123 -0.01102 -0.00001 -0.01103 3.78111

R16 2.84464 -0.00081 -0.00387 0.00000 -0.00387 2.84078

R17 2.48394 0.00175 0.00398 -0.00000 0.00398 2.48791

R18 2.54902 0.00045 0.00111 -0.00001 0.00110 2.55012

R19 2.80499 0.00062 0.00200 -0.00000 0.00199 2.80698

R20 2.04301 0.00015 0.00021 -0.00001 0.00020 2.04321

R21 2.48394 0.00175 0.00398 -0.00000 0.00398 2.48791

R22 2.54902 0.00045 0.00111 -0.00001 0.00110 2.55012

R23 2.84464 -0.00081 -0.00387 0.00000 -0.00387 2.84078

R24 2.80499 0.00062 0.00200 -0.00000 0.00199 2.80698

R25 2.80408 -0.00084 -0.00388 -0.00000 -0.00388 2.80020

R26 2.04301 0.00015 0.00021 -0.00001 0.00020 2.04321

R27 2.58096 0.00013 0.00224 0.00000 0.00225 2.58321

R28 2.49629 0.00057 0.00082 0.00001 0.00083 2.49711

R29 2.57895 -0.00029 -0.00109 0.00000 -0.00108 2.57787

R30 3.79214 -0.00123 -0.01102 -0.00001 -0.01103 3.78111

R31 2.58134 -0.00071 -0.00156 0.00000 -0.00156 2.57978

R32 2.55871 0.00056 0.00385 0.00000 0.00385 2.56256

R33 2.58454 -0.00062 -0.00284 -0.00001 -0.00285 2.58169

R34 3.80585 -0.00079 -0.00800 0.00001 -0.00799 3.79786

R35 2.77756 -0.00036 -0.00406 0.00001 -0.00405 2.77350

R36 2.59726 -0.00005 0.00060 0.00001 0.00060 2.59786

R37 2.81317 0.00004 0.00010 0.00000 0.00011 2.81328

R38 2.73083 0.00057 0.00156 0.00000 0.00156 2.73239

R39 2.04294 0.00003 0.00010 -0.00000 0.00010 2.04304

R40 2.58552 0.00021 0.00113 -0.00000 0.00113 2.58665

R41 2.06190 0.00023 0.00047 -0.00000 0.00047 2.06237

R42 2.06818 0.00047 0.00133 -0.00000 0.00133 2.06951

R43 2.06818 0.00047 0.00133 -0.00000 0.00133 2.06951

R44 2.06657 0.00075 0.00217 0.00000 0.00217 2.06875

R45 2.06657 0.00075 0.00217 0.00000 0.00217 2.06875

R46 2.06125 0.00012 0.00034 -0.00001 0.00034 2.06158

R47 2.06657 0.00075 0.00217 0.00000 0.00217 2.06875

R48 2.06657 0.00075 0.00217 0.00000 0.00217 2.06875

R49 2.06125 0.00012 0.00034 -0.00001 0.00034 2.06158

R50 2.06818 0.00047 0.00133 -0.00000 0.00133 2.06951

R51 2.06818 0.00047 0.00133 -0.00000 0.00133 2.06951

R52 2.06190 0.00023 0.00047 -0.00000 0.00047 2.06237

A1 1.88972 0.00051 0.00272 0.00000 0.00272 1.89244

A2 2.20381 -0.00013 0.00095 0.00000 0.00095 2.20477

A3 2.18965 -0.00038 -0.00367 -0.00000 -0.00367 2.18597

A4 1.91279 -0.00126 -0.00593 0.00000 -0.00593 1.90686

A5 2.19174 0.00035 0.00055 -0.00000 0.00055 2.19229

A6 2.17866 0.00091 0.00538 -0.00000 0.00538 2.18403

A7 1.88914 0.00146 0.00617 -0.00000 0.00617 1.89531

A8 2.22713 -0.00054 -0.00347 0.00000 -0.00347 2.22366

A9 2.16691 -0.00092 -0.00270 -0.00000 -0.00270 2.16421

A10 1.85555 -0.00104 -0.00366 -0.00000 -0.00367 1.85188

A11 2.16612 0.00134 0.00737 0.00000 0.00737 2.17349

A12 2.26152 -0.00030 -0.00371 0.00000 -0.00370 2.25781

A13 1.87757 0.00032 0.00071 -0.00000 0.00071 1.87828

A14 2.17952 0.00012 0.00141 0.00000 0.00141 2.18093

A15 2.22610 -0.00044 -0.00213 -0.00000 -0.00213 2.22397

A16 2.17177 -0.00057 -0.00354 -0.00001 -0.00354 2.16822

A17 2.23015 0.00041 0.00101 0.00001 0.00101 2.23116

A18 2.17152 -0.00061 -0.00319 -0.00000 -0.00319 2.16833

A19 1.88152 0.00021 0.00218 -0.00000 0.00218 1.88369

A20 1.91653 0.00006 -0.00242 -0.00000 -0.00242 1.91410

A21 2.18633 0.00018 0.00268 -0.00000 0.00268 2.18901

A22 2.18033 -0.00023 -0.00026 0.00000 -0.00026 2.18007

A23 1.88372 -0.00025 0.00081 -0.00000 0.00081 1.88453

A24 2.24524 0.00024 0.00160 -0.00000 0.00160 2.24684

A25 2.15422 0.00001 -0.00241 0.00000 -0.00241 2.15182

A26 1.85493 0.00046 0.00161 -0.00000 0.00161 1.85654

A27 2.15367 -0.00011 0.00074 0.00000 0.00074 2.15441

A28 2.27458 -0.00035 -0.00234 -0.00000 -0.00235 2.27224

A29 1.88808 -0.00047 -0.00218 0.00000 -0.00217 1.88591

A30 2.16445 0.00017 0.00027 -0.00001 0.00027 2.16471

A31 2.23066 0.00031 0.00190 0.00000 0.00191 2.23256

A32 2.17599 -0.00061 -0.00491 0.00000 -0.00490 2.17108

A33 1.85493 0.00046 0.00161 -0.00000 0.00161 1.85654

A34 2.27458 -0.00035 -0.00234 -0.00000 -0.00235 2.27224

A35 2.15367 -0.00011 0.00074 0.00000 0.00074 2.15441

A36 1.88808 -0.00047 -0.00218 0.00000 -0.00217 1.88591

A37 2.23066 0.00031 0.00190 0.00000 0.00191 2.23256

A38 2.16445 0.00017 0.00027 -0.00001 0.00027 2.16471

A39 1.88152 0.00021 0.00218 -0.00000 0.00218 1.88369

A40 2.17152 -0.00061 -0.00319 -0.00000 -0.00319 2.16833

A41 2.23015 0.00041 0.00101 0.00001 0.00101 2.23116

A42 1.91653 0.00006 -0.00242 -0.00000 -0.00242 1.91410

A43 2.18633 0.00018 0.00268 -0.00000 0.00268 2.18901

A44 2.18033 -0.00023 -0.00026 0.00000 -0.00026 2.18007

A45 2.15422 0.00001 -0.00241 0.00000 -0.00241 2.15182

A46 2.24524 0.00024 0.00160 -0.00000 0.00160 2.24684

A47 1.88372 -0.00025 0.00081 -0.00000 0.00081 1.88453

A48 2.17177 -0.00057 -0.00354 -0.00001 -0.00354 2.16822

A49 1.91279 -0.00126 -0.00593 0.00000 -0.00593 1.90686

A50 2.17866 0.00091 0.00538 -0.00000 0.00538 2.18403

A51 2.19174 0.00035 0.00055 -0.00000 0.00055 2.19229

A52 2.22713 -0.00054 -0.00347 0.00000 -0.00347 2.22366

A53 2.16691 -0.00092 -0.00270 -0.00000 -0.00270 2.16421

A54 1.88914 0.00146 0.00617 -0.00000 0.00617 1.89531

A55 1.85555 -0.00104 -0.00366 -0.00000 -0.00367 1.85188

A56 2.16612 0.00134 0.00737 0.00000 0.00737 2.17349

A57 2.26152 -0.00030 -0.00371 0.00000 -0.00370 2.25781

A58 1.87757 0.00032 0.00071 -0.00000 0.00071 1.87828

A59 2.22610 -0.00044 -0.00213 -0.00000 -0.00213 2.22397

A60 2.17952 0.00012 0.00141 0.00000 0.00141 2.18093

A61 1.88972 0.00051 0.00272 0.00000 0.00272 1.89244

A62 2.20381 -0.00013 0.00095 0.00000 0.00095 2.20477

A63 2.18965 -0.00038 -0.00367 -0.00000 -0.00367 2.18597

A64 2.17599 -0.00061 -0.00491 0.00000 -0.00490 2.17108

A65 1.57233 -0.00038 -0.00206 0.00000 -0.00206 1.57028

A66 1.56926 0.00038 0.00206 -0.00000 0.00206 1.57132

A67 1.56926 0.00038 0.00206 -0.00000 0.00206 1.57132

A68 1.57233 -0.00038 -0.00206 0.00000 -0.00206 1.57028

A69 1.94449 -0.00005 -0.00141 -0.00000 -0.00141 1.94307

A70 1.94100 -0.00012 -0.00044 -0.00000 -0.00044 1.94056

A71 1.94100 -0.00012 -0.00044 -0.00000 -0.00044 1.94056

A72 1.88846 0.00011 0.00101 -0.00000 0.00101 1.88947

A73 1.88846 0.00011 0.00101 -0.00000 0.00101 1.88947

A74 1.85711 0.00009 0.00042 0.00001 0.00043 1.85754

A75 1.93206 0.00027 0.00176 -0.00000 0.00176 1.93382

A76 1.93206 0.00027 0.00176 -0.00000 0.00176 1.93382

A77 1.94762 -0.00033 -0.00231 -0.00001 -0.00232 1.94530

A78 1.85900 -0.00021 -0.00123 0.00001 -0.00123 1.85778

A79 1.89518 0.00000 0.00001 0.00000 0.00002 1.89520

A80 1.89518 0.00000 0.00001 0.00000 0.00002 1.89520

A81 1.93206 0.00027 0.00176 -0.00000 0.00176 1.93382

A82 1.93206 0.00027 0.00176 -0.00000 0.00176 1.93382

A83 1.94762 -0.00033 -0.00231 -0.00001 -0.00232 1.94530

A84 1.85900 -0.00021 -0.00123 0.00001 -0.00123 1.85778

A85 1.89518 0.00000 0.00001 0.00000 0.00002 1.89520

A86 1.89518 0.00000 0.00001 0.00000 0.00002 1.89520

A87 1.94100 -0.00012 -0.00044 -0.00000 -0.00044 1.94056

A88 1.94100 -0.00012 -0.00044 -0.00000 -0.00044 1.94056

A89 1.94449 -0.00005 -0.00141 -0.00000 -0.00141 1.94307

A90 1.85711 0.00009 0.00042 0.00001 0.00043 1.85754

A91 1.88846 0.00011 0.00101 -0.00000 0.00101 1.88947

A92 1.88846 0.00011 0.00101 -0.00000 0.00101 1.88947

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 1.03321 -0.00002 -0.00002 0.00000 -0.00002 1.03319

D31 -1.03321 0.00002 0.00002 -0.00000 0.00002 -1.03319

D32 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D33 -2.10838 -0.00002 -0.00002 0.00000 -0.00002 -2.10840

D34 2.10838 0.00002 0.00002 -0.00000 0.00002 2.10840

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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D80 2.11292 -0.00004 -0.00034 -0.00000 -0.00034 2.11257

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D115 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

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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

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D126 -1.03321 0.00002 0.00002 -0.00000 0.00002 -1.03319

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D129 2.10838 0.00002 0.00002 -0.00000 0.00002 2.10840

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

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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

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D136 3.14159 -0.00000 0.00000 -0.00000 0.00000 3.14159

Item Value Threshold Converged?

Maximum Force 0.001753 0.000450 NO

RMS Force 0.000405 0.000300 NO

Maximum Displacement 0.015530 0.001800 NO

RMS Displacement 0.004267 0.001200 NO

Predicted change in Energy=-9.930087D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Sep 17 14:40:58 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

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1 6 0 -2.073315 -2.191841 0.000000

2 7 0 -0.746589 -1.865919 0.000000

3 6 0 -0.006905 -3.002466 0.000000

4 6 0 -0.917541 -4.153471 0.000000

5 6 0 -2.189957 -3.633049 0.000000

6 7 0 1.354326 -3.106004 0.000000

7 6 0 2.178365 -2.073000 0.000000

8 7 0 1.857303 -0.744263 0.000000

9 6 0 2.998067 0.003772 0.000000

10 6 0 4.170114 -0.937577 0.000000

11 6 0 3.655909 -2.185232 0.000000

12 7 0 -3.123801 -1.314302 0.000000

13 6 0 -4.170114 0.937577 0.000000

14 6 0 -3.655909 2.185232 0.000000

15 6 0 -2.178365 2.073000 0.000000

16 7 0 -1.857303 0.744263 0.000000

17 6 0 -2.998067 -0.003772 0.000000

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20 6 0 0.006905 3.002466 0.000000

21 6 0 0.917541 4.153471 0.000000

22 6 0 2.189957 3.633049 0.000000

23 6 0 2.073315 2.191841 0.000000

24 7 0 3.123801 1.314302 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.479341 -5.576242 0.000000

27 1 0 -3.123102 -4.179016 0.000000

28 6 0 5.584470 -0.483720 0.000000

29 1 0 4.191364 -3.124554 0.000000

30 6 0 -5.584470 0.483720 0.000000

31 1 0 -4.191364 3.124554 0.000000

32 6 0 0.479341 5.576242 0.000000

33 1 0 3.123102 4.179016 0.000000

34 1 0 -1.334061 -6.254859 0.000000

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36 1 0 0.136886 -5.800576 -0.877080

37 1 0 5.793373 0.137541 0.876832

38 1 0 5.793373 0.137541 -0.876832

39 1 0 6.274693 -1.328556 0.000000

40 1 0 -5.793373 -0.137541 0.876832

41 1 0 -5.793373 -0.137541 -0.876832

42 1 0 -6.274693 1.328556 0.000000

43 1 0 -0.136886 5.800576 0.877080

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45 1 0 1.334061 6.254859 0.000000

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Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.366172 0.000000

3 C 2.219721 1.356050 0.000000

4 C 2.276797 2.293931 1.467676 0.000000

5 C 1.445920 2.281679 2.272301 1.374729 0.000000

6 N 3.547452 2.439601 1.365162 2.501713 3.583255

7 C 4.253341 2.932276 2.374724 3.730013 4.638533

8 N 4.188704 2.835202 2.928268 4.395732 4.972464

9 C 5.526267 4.185474 4.250567 5.710924 6.335776

10 C 6.368170 5.003578 4.659534 6.018822 6.907682

11 C 5.729227 4.414063 3.752875 4.978997 6.022484

12 N 1.368794 2.440372 3.544706 3.595617 2.499730

13 C 3.766939 4.424943 5.732038 6.041358 4.981129

14 C 4.654393 4.987581 6.342511 6.904913 6.000117

15 C 4.266135 4.191070 5.520471 6.352844 5.706061

16 N 2.944039 2.836677 4.178750 4.987078 4.389933

17 C 2.375460 2.921770 4.235471 4.642046 3.718157

18 N 5.346411 5.008928 6.255314 7.272603 6.790664

19 N 4.941384 4.019478 4.926350 6.245189 6.233936

20 C 5.595367 4.926350 6.004948 7.215403 6.989725

21 C 7.014856 6.245189 7.215403 8.507221 8.383701

22 C 7.218367 6.233936 6.989725 8.383701 8.484092

23 C 6.034170 4.941384 5.595367 7.014856 7.218367

24 N 6.269215 5.009364 5.332524 6.799191 7.260324

25 Zn 3.017085 2.009739 3.002474 4.253611 4.242046

26 C 3.740979 3.719935 2.616776 1.488723 2.588862

27 H 2.247425 3.316358 3.330909 2.205708 1.081129

28 C 7.845976 6.480184 6.132499 7.466138 8.388086

29 H 6.333732 5.095836 4.200044 5.211486 6.401549

30 C 4.414390 5.378279 6.577440 6.579040 5.335776

31 H 5.722778 6.063934 7.419574 7.980449 7.047753

32 C 8.176745 7.542457 8.592477 9.829475 9.588336

33 H 8.221348 7.177448 7.833941 9.260515 9.447590

34 H 4.129723 4.428083 3.512749 2.142270 2.757979

35 H 4.321716 4.126902 2.935876 2.143371 3.298734

36 H 4.321716 4.126902 2.935876 2.143371 3.298734

37 H 8.251038 6.895926 6.653698 8.013613 8.872415

38 H 8.251038 6.895926 6.653698 8.013613 8.872415

39 H 8.392526 7.041815 6.500803 7.727120 8.772741

40 H 4.339103 5.406122 6.516122 6.377324 5.096275

41 H 4.339103 5.406122 6.516122 6.377324 5.096275

42 H 5.481311 6.384716 7.618590 7.664965 6.426709

43 H 8.270294 7.740553 8.847582 10.023061 9.694207

44 H 8.270294 7.740553 8.847582 10.023061 9.694207

45 H 9.108070 8.383087 9.353943 10.649086 10.497115

6 7 8 9 10

6 N 0.000000

7 C 1.321415 0.000000

8 N 2.414707 1.366977 0.000000

9 C 3.517470 2.232688 1.364147 0.000000

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11 C 2.478932 1.481800 2.304642 2.285716 1.349463

12 N 4.823258 5.356173 5.013616 6.262155 7.303638

13 C 6.846166 7.026149 6.257663 7.228749 8.548428

14 C 7.286949 7.222970 6.243192 7.002440 8.426066

15 C 6.269130 6.014185 4.921747 5.574689 7.026149

16 N 5.013892 4.921747 4.001750 4.911511 6.257663

17 C 5.344826 5.574689 4.911511 5.996139 7.228749

18 N 6.776860 6.269130 5.013892 5.344826 6.846166

19 N 5.008928 4.191070 2.836677 2.921770 4.424943

20 C 6.255314 5.520471 4.178750 4.235471 5.732038

21 C 7.272603 6.352844 4.987078 4.642046 6.041358

22 C 6.790664 5.706061 4.389933 3.718157 4.981129

23 C 5.346411 4.266135 2.944039 2.375460 3.766939

24 N 4.761318 3.516769 2.416962 1.316548 2.483089

25 Zn 3.388430 3.007093 2.000875 2.998069 4.274214

26 C 3.076428 4.397284 5.367302 6.574870 6.567697

27 H 4.604206 5.704459 6.049956 7.413800 7.981098

28 C 4.976996 3.758638 3.736262 2.631944 1.485391

29 H 2.837099 2.271108 3.333711 3.348191 2.187080

30 C 7.812362 8.173031 7.542408 8.595946 9.857586

31 H 8.341135 8.221194 7.180120 7.837551 9.295980

32 C 8.726224 7.835661 6.468969 6.115259 7.486765

33 H 7.496672 6.322993 5.083397 4.177116 5.222621

34 H 4.140375 5.461234 6.368004 7.611688 7.653067

35 H 3.084177 4.339554 5.412523 6.530397 6.378476

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37 H 5.567276 4.327079 4.127840 2.932655 2.135341

38 H 5.567276 4.327079 4.127840 2.932655 2.135341

39 H 5.231571 4.163424 4.455865 3.537142 2.140587

40 H 7.789108 8.250058 7.724622 8.836188 10.033941

41 H 7.789108 8.250058 7.724622 8.836188 10.033941

42 H 8.824242 9.111793 8.392016 9.366917 10.687814

43 H 9.073045 8.253658 6.897896 6.648318 8.045013

44 H 9.073045 8.253658 6.897896 6.648318 8.045013

45 H 9.360885 8.370549 7.018653 6.468771 7.731387

11 12 13 14 15

11 C 0.000000

12 N 6.835422 0.000000

13 C 8.426066 2.483089 0.000000

14 C 8.518429 3.539757 1.349463 0.000000

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16 N 6.243192 2.416962 2.320876 2.304642 1.366977

17 C 7.002440 1.316548 1.503275 2.285716 2.232688

18 N 7.286949 4.761318 3.553975 2.478932 1.321415

19 N 4.987581 5.009364 5.003578 4.414063 2.932276

20 C 6.342511 5.332524 4.659534 3.752875 2.374724

21 C 6.904913 6.799191 6.018822 4.978997 3.730013

22 C 6.000117 7.260324 6.907682 6.022484 4.638533

23 C 4.654393 6.269215 6.368170 5.729227 4.253341

24 N 3.539757 6.778060 7.303638 6.835422 5.356173

25 Zn 4.259215 3.389030 4.274214 4.259215 3.007093

26 C 5.347825 5.015705 7.486765 8.386362 7.835661

27 H 7.066127 2.864714 5.222621 6.386513 6.322993

28 C 2.571865 8.747791 9.857586 9.618103 8.173031

29 H 1.081221 7.535825 9.295980 9.474889 8.221194

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32 C 8.386362 7.775746 6.567697 5.347825 4.397284

33 H 6.386513 8.318674 7.981098 7.066127 5.704459

34 H 6.439073 5.254738 7.731387 8.753635 8.370549

35 H 5.120889 5.614980 8.045013 8.884126 8.253658

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37 H 3.276105 9.077042 10.033941 9.708285 8.250058

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43 H 8.884126 7.766107 6.378476 5.120889 4.339554

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16 17 18 19 20

16 N 0.000000

17 C 1.364147 0.000000

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21 C 4.395732 5.710924 2.501713 2.293931 1.467676

22 C 4.972464 6.335776 3.583255 2.281679 2.272301

23 C 4.188704 5.526267 3.547452 1.366172 2.219721

24 N 5.013616 6.262155 4.823258 2.440372 3.544706

25 Zn 2.000875 2.998069 3.388430 2.009739 3.002474

26 C 6.468969 6.115259 8.726224 7.542457 8.592477

27 H 5.083397 4.177116 7.496672 7.177448 7.833941

28 C 7.542408 8.595946 7.812362 5.378279 6.577440

29 H 7.180120 7.837551 8.341135 6.063934 7.419574

30 C 3.736262 2.631944 4.976996 6.480184 6.132499

31 H 3.333711 3.348191 2.837099 5.095836 4.200044

32 C 5.367302 6.574870 3.076428 3.719935 2.616776

33 H 6.049956 7.413800 4.604206 3.316358 3.330909

34 H 7.018653 6.468771 9.360885 8.383087 9.353943

35 H 6.897896 6.648318 9.073045 7.740553 8.847582

36 H 6.897896 6.648318 9.073045 7.740553 8.847582

37 H 7.724622 8.836188 7.789108 5.406122 6.516122

38 H 7.724622 8.836188 7.789108 5.406122 6.516122

39 H 8.392016 9.366917 8.824242 6.384716 7.618590

40 H 4.127840 2.932655 5.567276 6.895926 6.653698

41 H 4.127840 2.932655 5.567276 6.895926 6.653698

42 H 4.455865 3.537142 5.231571 7.041815 6.500803

43 H 5.412523 6.530397 3.084177 4.126902 2.935876

44 H 5.412523 6.530397 3.084177 4.126902 2.935876

45 H 6.368004 7.611688 4.140375 4.428083 3.512749

21 22 23 24 25

21 C 0.000000

22 C 1.374729 0.000000

23 C 2.276797 1.445920 0.000000

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25 Zn 4.253611 4.242046 3.017085 3.389030 0.000000

26 C 9.829475 9.588336 8.176745 7.775746 5.596806

27 H 9.260515 9.447590 8.221348 8.318674 5.217082

28 C 6.579040 5.335776 4.414390 3.047585 5.605380

29 H 7.980449 7.047753 5.722778 4.565428 5.227846

30 C 7.466138 8.388086 7.845976 8.747791 5.605380

31 H 5.211486 6.401549 6.333732 7.535825 5.227846

32 C 1.488723 2.588862 3.740979 5.015705 5.596806

33 H 2.205708 1.081129 2.247425 2.864714 5.217082

34 H 10.649086 10.497115 9.108070 8.784346 6.395544

35 H 10.023061 9.694207 8.270294 7.766107 5.868108

36 H 10.023061 9.694207 8.270294 7.766107 5.868108

37 H 6.377324 5.096275 4.339103 3.046345 5.860966

38 H 6.377324 5.096275 4.339103 3.046345 5.860966

39 H 7.664965 6.426709 5.481311 4.112519 6.413800

40 H 8.013613 8.872415 8.251038 9.077042 5.860966

41 H 8.013613 8.872415 8.251038 9.077042 5.860966

42 H 7.727120 8.772741 8.392526 9.398505 6.413800

43 H 2.143371 3.298734 4.321716 5.614980 5.868108

44 H 2.143371 3.298734 4.321716 5.614980 5.868108

45 H 2.142270 2.757979 4.129723 5.254738 6.395544

26 27 28 29 30

26 C 0.000000

27 H 2.990269 0.000000

28 C 7.918559 9.459229 0.000000

29 H 5.275060 7.390081 2.985758 0.000000

30 C 7.923729 5.272518 11.210760 10.420488 0.000000

31 H 9.459544 7.381282 10.420488 10.455692 2.985758

32 C 11.193612 10.399166 7.923729 9.459544 7.918559

33 H 10.399166 10.434164 5.272518 7.381282 9.459229

34 H 1.091360 2.740399 9.009557 6.350522 7.967084

35 H 1.095140 3.745163 7.662532 4.936512 8.543744

36 H 1.095140 3.745163 7.662532 4.936512 8.543744

37 H 8.530128 9.945101 1.094733 3.738520 11.416829

38 H 8.530128 9.945101 1.094733 3.738520 11.416829

39 H 7.978710 9.820574 1.090942 2.750613 11.996836

40 H 7.654230 4.922673 11.416829 10.458779 1.094733

41 H 7.654230 4.922673 11.416829 10.458779 1.094733

42 H 9.014562 6.345540 11.996836 11.374029 1.090942

43 H 11.415714 10.453661 8.543744 9.957960 7.662532

44 H 11.415714 10.453661 8.543744 9.957960 7.662532

45 H 11.969268 11.346015 7.967084 9.804977 9.009557

31 32 33 34 35

31 H 0.000000

32 C 5.275060 0.000000

33 H 7.390081 2.990269 0.000000

34 H 9.804977 11.969268 11.346015 0.000000

35 H 9.957960 11.415714 10.453661 1.771815 0.000000

36 H 9.957960 11.415714 10.453661 1.771815 1.754159

37 H 10.458779 7.654230 4.922673 9.614153 8.201042

38 H 10.458779 7.654230 4.922673 9.614153 8.386494

39 H 11.374029 9.014562 6.345540 9.064304 7.644665

40 H 3.738520 8.530128 9.945101 7.620753 8.199875

41 H 3.738520 8.530128 9.945101 7.620753 8.385353

42 H 2.750613 7.978710 9.820574 9.050857 9.628195

43 H 4.936512 1.095140 3.745163 12.146440 11.604382

44 H 4.936512 1.095140 3.745163 12.146440 11.736216

45 H 6.350522 1.091360 2.740399 12.791087 12.146440

36 37 38 39 40

36 H 0.000000

37 H 8.386494 0.000000

38 H 8.201042 1.753664 0.000000

39 H 7.644665 1.774808 1.774808 0.000000

40 H 8.385353 11.590011 11.721932 12.158354 0.000000

41 H 8.199875 11.721932 11.590011 12.158354 1.753664

42 H 9.628195 12.158354 12.158354 12.827600 1.774808

43 H 11.736216 8.199875 8.385353 9.628195 8.201042

44 H 11.604382 8.385353 8.199875 9.628195 8.386494

45 H 12.146440 7.620753 7.620753 9.050857 9.614153

41 42 43 44 45

41 H 0.000000

42 H 1.774808 0.000000

43 H 8.386494 7.644665 0.000000

44 H 8.201042 7.644665 1.754159 0.000000

45 H 9.614153 9.064304 1.771815 1.771815 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=0 Diff= 8.77D-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 2.805774 -1.109249 0.000000

2 7 0 2.009739 0.001045 0.000000

3 6 0 2.789593 1.110414 0.000000

4 6 0 4.196737 0.693257 0.000000

5 6 0 4.186956 -0.681437 0.000000

6 7 0 2.379367 2.412482 0.000000

7 6 0 1.113969 2.793148 0.000000

8 7 0 0.000000 2.000875 0.000000

9 6 0 -1.118688 2.781538 0.000000

10 6 0 -0.680850 4.219639 0.000000

11 6 0 0.668548 4.206418 0.000000

12 7 0 2.381951 -2.410775 0.000000

13 6 0 0.680850 -4.219639 0.000000

14 6 0 -0.668548 -4.206418 0.000000

15 6 0 -1.113969 -2.793148 0.000000

16 7 0 -0.000000 -2.000875 0.000000

17 6 0 1.118688 -2.781538 0.000000

18 7 0 -2.379367 -2.412482 0.000000

19 7 0 -2.009739 -0.001045 0.000000

20 6 0 -2.789593 -1.110414 0.000000

21 6 0 -4.196737 -0.693257 0.000000

22 6 0 -4.186956 0.681437 0.000000

23 6 0 -2.805774 1.109249 0.000000

24 7 0 -2.381951 2.410775 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 5.354420 1.629241 0.000000

27 1 0 5.040848 -1.344542 0.000000

28 6 0 -1.628236 5.363686 0.000000

29 1 0 1.341297 5.052850 0.000000

30 6 0 1.628236 -5.363686 0.000000

31 1 0 -1.341297 -5.052850 0.000000

32 6 0 -5.354420 -1.629241 0.000000

33 1 0 -5.040848 1.344542 0.000000

34 1 0 6.302272 1.088275 0.000000

35 1 0 5.333440 2.284696 0.877080

36 1 0 5.333440 2.284696 -0.877080

37 1 0 -2.282625 5.326511 0.876832

38 1 0 -2.282625 5.326511 -0.876832

39 1 0 -1.100763 6.318635 0.000000

40 1 0 2.282625 -5.326511 0.876832

41 1 0 2.282625 -5.326511 -0.876832

42 1 0 1.100763 -6.318635 0.000000

43 1 0 -5.333440 -2.284696 0.877080

44 1 0 -5.333440 -2.284696 -0.877080

45 1 0 -6.302272 -1.088275 0.000000

---------------------------------------------------------------------

Rotational constants (GHZ): 0.1829582 0.1818963 0.0914175

Leave Link 202 at Tue Sep 17 14:40:58 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 101 beta electrons

nuclear repulsion energy 2761.7116016960 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= -0.1142196075 Hartrees.

Nuclear repulsion after empirical dispersion term = 2761.5973820885 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 = 3494

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.19D-06

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 122

GePol: Fraction of low-weight points (<1% of avg) = 3.49%

GePol: Cavity surface area = 382.087 Ang\*\*2

GePol: Cavity volume = 379.322 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0107106116 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2761.5866714769 Hartrees.

Leave Link 301 at Tue Sep 17 14:40:58 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= 15325 LenP2D= 41264.

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 14:40:59 2019, MaxMem= 2415919104 cpu: 12.8

(Enter /home/blab/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Tue Sep 17 14:40:59 2019, MaxMem= 2415919104 cpu: 1.2

(Enter /home/blab/g09/l401.exe)

Initial guess from the checkpoint file: "ZntAzP3.chk"

B after Tr= 0.000000 0.000000 -0.000000

Rot= 1.000000 0.000000 -0.000000 -0.000402 Ang= -0.05 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 3-BU.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0180 S= 1.0060

Leave Link 401 at Tue Sep 17 14:41:00 2019, MaxMem= 2415919104 cpu: 22.6

(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= 36624108.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.66D-15 for 3479.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.08D-15 for 1762 189.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.33D-15 for 3479.

Iteration 1 A^-1\*A deviation from orthogonality is 4.66D-12 for 1982 1968.

E= -1275.84256563989

DIIS: error= 5.82D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.84256563989 IErMin= 1 ErrMin= 5.82D-04

ErrMax= 5.82D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.82D-04 BMatP= 3.82D-04

IDIUse=3 WtCom= 9.94D-01 WtEn= 5.82D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.303 Goal= None Shift= 0.000

Gap= 0.393 Goal= None Shift= 0.000

RMSDP=2.91D-05 MaxDP=8.15D-04 OVMax= 4.47D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.90D-05 CP: 1.00D+00

E= -1275.84266033561 Delta-E= -0.000094695716 Rises=F Damp=F

DIIS: error= 1.91D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.84266033561 IErMin= 2 ErrMin= 1.91D-04

ErrMax= 1.91D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.54D-05 BMatP= 3.82D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.91D-03

Coeff-Com: 0.149D+00 0.851D+00

Coeff-En: 0.000D+00 0.100D+01

Coeff: 0.149D+00 0.851D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.13D-05 MaxDP=4.92D-04 DE=-9.47D-05 OVMax= 3.25D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.12D-05 CP: 1.00D+00 9.80D-01

E= -1275.84265252520 Delta-E= 0.000007810403 Rises=F Damp=F

DIIS: error= 2.39D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1275.84266033561 IErMin= 2 ErrMin= 1.91D-04

ErrMax= 2.39D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.03D-04 BMatP= 5.54D-05

IDIUse=3 WtCom= 3.93D-01 WtEn= 6.07D-01

Coeff-Com: -0.125D-01 0.585D+00 0.427D+00

Coeff-En: 0.000D+00 0.602D+00 0.398D+00

Coeff: -0.493D-02 0.595D+00 0.409D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=6.69D-06 MaxDP=2.82D-04 DE= 7.81D-06 OVMax= 1.23D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 3.88D-06 CP: 1.00D+00 1.04D+00 5.46D-01

E= -1275.84267415649 Delta-E= -0.000021631284 Rises=F Damp=F

DIIS: error= 4.68D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.84267415649 IErMin= 4 ErrMin= 4.68D-05

ErrMax= 4.68D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.26D-06 BMatP= 5.54D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.997D-02 0.219D+00 0.166D+00 0.625D+00

Coeff: -0.997D-02 0.219D+00 0.166D+00 0.625D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.08D-06 MaxDP=1.04D-04 DE=-2.16D-05 OVMax= 1.35D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.52D-06 CP: 1.00D+00 1.06D+00 6.15D-01 1.28D+00

E= -1275.84267500429 Delta-E= -0.000000847804 Rises=F Damp=F

DIIS: error= 3.64D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.84267500429 IErMin= 5 ErrMin= 3.64D-05

ErrMax= 3.64D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.16D-07 BMatP= 1.26D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.201D-02 0.274D-02 0.707D-02 0.335D+00 0.658D+00

Coeff: -0.201D-02 0.274D-02 0.707D-02 0.335D+00 0.658D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.94D-06 MaxDP=8.82D-05 DE=-8.48D-07 OVMax= 1.36D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 6.47D-07 CP: 1.00D+00 1.07D+00 6.74D-01 1.68D+00 1.37D+00

E= -1275.84267564506 Delta-E= -0.000000640769 Rises=F Damp=F

DIIS: error= 3.22D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.84267564506 IErMin= 6 ErrMin= 3.22D-05

ErrMax= 3.22D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.70D-07 BMatP= 5.16D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.337D-02-0.754D-01-0.551D-01-0.929D-01 0.834D-01 0.114D+01

Coeff: 0.337D-02-0.754D-01-0.551D-01-0.929D-01 0.834D-01 0.114D+01

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.91D-06 MaxDP=1.41D-04 DE=-6.41D-07 OVMax= 2.15D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.47D-07 CP: 1.00D+00 1.09D+00 7.67D-01 2.24D+00 2.26D+00

CP: 1.85D+00

E= -1275.84267629761 Delta-E= -0.000000652553 Rises=F Damp=F

DIIS: error= 2.12D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.84267629761 IErMin= 7 ErrMin= 2.12D-05

ErrMax= 2.12D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.85D-07 BMatP= 1.70D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.461D-02-0.721D-01-0.585D-01-0.341D+00-0.529D+00 0.106D+01

Coeff-Com: 0.932D+00

Coeff: 0.461D-02-0.721D-01-0.585D-01-0.341D+00-0.529D+00 0.106D+01

Coeff: 0.932D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.70D-06 MaxDP=1.75D-04 DE=-6.53D-07 OVMax= 2.72D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 6.54D-07 CP: 1.00D+00 1.11D+00 8.85D-01 2.95D+00 3.00D+00

CP: 3.00D+00 1.65D+00

E= -1275.84267681808 Delta-E= -0.000000520467 Rises=F Damp=F

DIIS: error= 1.24D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.84267681808 IErMin= 8 ErrMin= 1.24D-05

ErrMax= 1.24D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.40D-08 BMatP= 1.70D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.564D-03 0.970D-02 0.937D-03-0.880D-01-0.274D+00 0.124D-01

Coeff-Com: 0.385D+00 0.953D+00

Coeff: 0.564D-03 0.970D-02 0.937D-03-0.880D-01-0.274D+00 0.124D-01

Coeff: 0.385D+00 0.953D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.92D-06 MaxDP=9.97D-05 DE=-5.20D-07 OVMax= 1.48D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.31D-06 CP: 1.00D+00 1.13D+00 9.41D-01 3.00D+00 3.00D+00

CP: 3.00D+00 2.40D+00 2.42D+00

E= -1275.84267693638 Delta-E= -0.000000118299 Rises=F Damp=F

DIIS: error= 7.26D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.84267693638 IErMin= 9 ErrMin= 7.26D-06

ErrMax= 7.26D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.61D-08 BMatP= 3.40D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.124D-02 0.313D-01 0.191D-01 0.599D-01 0.199D-01-0.335D+00

Coeff-Com: -0.881D-01 0.656D+00 0.638D+00

Coeff: -0.124D-02 0.313D-01 0.191D-01 0.599D-01 0.199D-01-0.335D+00

Coeff: -0.881D-01 0.656D+00 0.638D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=6.44D-07 MaxDP=3.34D-05 DE=-1.18D-07 OVMax= 4.84D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.72D-07 CP: 1.00D+00 1.13D+00 9.57D-01 3.00D+00 3.00D+00

CP: 3.00D+00 2.71D+00 3.00D+00 1.31D+00

E= -1275.84267696431 Delta-E= -0.000000027925 Rises=F Damp=F

DIIS: error= 3.56D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.84267696431 IErMin=10 ErrMin= 3.56D-06

ErrMax= 3.56D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.33D-09 BMatP= 2.61D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.548D-03 0.657D-02 0.413D-02 0.493D-01 0.117D+00-0.133D+00

Coeff-Com: -0.200D+00-0.143D-01 0.152D+00 0.102D+01

Coeff: -0.548D-03 0.657D-02 0.413D-02 0.493D-01 0.117D+00-0.133D+00

Coeff: -0.200D+00-0.143D-01 0.152D+00 0.102D+01

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=5.01D-07 MaxDP=2.81D-05 DE=-2.79D-08 OVMax= 3.87D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 3.13D-07 CP: 1.00D+00 1.13D+00 9.71D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.55D+00 1.45D+00

E= -1275.84267697638 Delta-E= -0.000000012074 Rises=F Damp=F

DIIS: error= 2.62D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.84267697638 IErMin=11 ErrMin= 2.62D-06

ErrMax= 2.62D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.40D-09 BMatP= 4.33D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.291D-05-0.575D-02-0.341D-02 0.168D-01 0.768D-01 0.302D-01

Coeff-Com: -0.128D+00-0.227D+00-0.191D+00 0.718D+00 0.714D+00

Coeff: -0.291D-05-0.575D-02-0.341D-02 0.168D-01 0.768D-01 0.302D-01

Coeff: -0.128D+00-0.227D+00-0.191D+00 0.718D+00 0.714D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.91D-07 MaxDP=1.53D-05 DE=-1.21D-08 OVMax= 2.15D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.04D-07 CP: 1.00D+00 1.13D+00 9.77D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.68D+00 2.03D+00

CP: 1.54D+00

E= -1275.84267698081 Delta-E= -0.000000004426 Rises=F Damp=F

DIIS: error= 1.04D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.84267698081 IErMin=12 ErrMin= 1.04D-06

ErrMax= 1.04D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.56D-10 BMatP= 3.40D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.173D-03-0.544D-02-0.331D-02-0.530D-02 0.344D-02 0.637D-01

Coeff-Com: -0.214D-01-0.104D+00-0.170D+00 0.107D+00 0.344D+00 0.791D+00

Coeff: 0.173D-03-0.544D-02-0.331D-02-0.530D-02 0.344D-02 0.637D-01

Coeff: -0.214D-01-0.104D+00-0.170D+00 0.107D+00 0.344D+00 0.791D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.60D-07 MaxDP=8.57D-06 DE=-4.43D-09 OVMax= 1.22D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 3.38D-08 CP: 1.00D+00 1.13D+00 9.81D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.76D+00 2.27D+00

CP: 1.83D+00 1.32D+00

E= -1275.84267698192 Delta-E= -0.000000001115 Rises=F Damp=F

DIIS: error= 5.64D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.84267698192 IErMin=13 ErrMin= 5.64D-07

ErrMax= 5.64D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.74D-10 BMatP= 6.56D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.111D-03-0.147D-02-0.937D-03-0.841D-02-0.245D-01 0.276D-01

Coeff-Com: 0.197D-01 0.201D-01-0.408D-01-0.163D+00-0.432D-01 0.479D+00

Coeff-Com: 0.736D+00

Coeff: 0.111D-03-0.147D-02-0.937D-03-0.841D-02-0.245D-01 0.276D-01

Coeff: 0.197D-01 0.201D-01-0.408D-01-0.163D+00-0.432D-01 0.479D+00

Coeff: 0.736D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.22D-07 MaxDP=6.14D-06 DE=-1.12D-09 OVMax= 9.30D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 2.08D-08 CP: 1.00D+00 1.13D+00 9.85D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.82D+00 2.43D+00

CP: 2.02D+00 1.59D+00 1.00D+00

E= -1275.84267698227 Delta-E= -0.000000000350 Rises=F Damp=F

DIIS: error= 1.98D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.84267698227 IErMin=14 ErrMin= 1.98D-07

ErrMax= 1.98D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.18D-11 BMatP= 2.74D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.112D-04 0.767D-03 0.450D-03-0.241D-02-0.131D-01-0.189D-02

Coeff-Com: 0.131D-01 0.408D-01 0.227D-01-0.118D+00-0.107D+00 0.722D-01

Coeff-Com: 0.393D+00 0.700D+00

Coeff: 0.112D-04 0.767D-03 0.450D-03-0.241D-02-0.131D-01-0.189D-02

Coeff: 0.131D-01 0.408D-01 0.227D-01-0.118D+00-0.107D+00 0.722D-01

Coeff: 0.393D+00 0.700D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.45D-08 MaxDP=1.26D-06 DE=-3.50D-10 OVMax= 1.78D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 7.23D-09 CP: 1.00D+00 1.13D+00 9.85D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.83D+00 2.46D+00

CP: 2.06D+00 1.63D+00 1.12D+00 1.18D+00

E= -1275.84267698228 Delta-E= -0.000000000008 Rises=F Damp=F

DIIS: error= 7.33D-08 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.84267698228 IErMin=15 ErrMin= 7.33D-08

ErrMax= 7.33D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.93D-12 BMatP= 4.18D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.123D-04 0.547D-03 0.320D-03 0.315D-04-0.183D-02-0.572D-02

Coeff-Com: 0.282D-02 0.138D-01 0.173D-01-0.275D-01-0.351D-01-0.509D-01

Coeff-Com: 0.417D-01 0.279D+00 0.765D+00

Coeff: -0.123D-04 0.547D-03 0.320D-03 0.315D-04-0.183D-02-0.572D-02

Coeff: 0.282D-02 0.138D-01 0.173D-01-0.275D-01-0.351D-01-0.509D-01

Coeff: 0.417D-01 0.279D+00 0.765D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.37D-08 MaxDP=6.85D-07 DE=-7.73D-12 OVMax= 1.00D-05

Cycle 16 Pass 1 IDiag 1:

RMSU= 2.34D-09 CP: 1.00D+00 1.13D+00 9.86D-01 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.84D+00 2.47D+00

CP: 2.08D+00 1.66D+00 1.16D+00 1.31D+00 9.86D-01

E= -1275.84267698230 Delta-E= -0.000000000025 Rises=F Damp=F

DIIS: error= 3.28D-08 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1275.84267698230 IErMin=16 ErrMin= 3.28D-08

ErrMax= 3.28D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.29D-12 BMatP= 4.93D-12

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.607D-05 0.118D-03 0.669D-04 0.372D-03 0.125D-02-0.207D-02

Coeff-Com: -0.357D-03-0.322D-03 0.458D-02 0.408D-02 0.517D-04-0.322D-01

Coeff-Com: -0.268D-01 0.302D-01 0.368D+00 0.653D+00

Coeff: -0.607D-05 0.118D-03 0.669D-04 0.372D-03 0.125D-02-0.207D-02

Coeff: -0.357D-03-0.322D-03 0.458D-02 0.408D-02 0.517D-04-0.322D-01

Coeff: -0.268D-01 0.302D-01 0.368D+00 0.653D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=4.26D-09 MaxDP=2.17D-07 DE=-2.50D-11 OVMax= 3.18D-06

Error on total polarization charges = 0.06464

SCF Done: E(UB3LYP) = -1275.84267698 A.U. after 16 cycles

NFock= 16 Conv=0.43D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0178 S= 1.0059

<L.S>= 0.000000000000E+00

KE= 1.320804808098D+03 PE=-8.575129362439D+03 EE= 3.216895205881D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.72

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0178, after 2.0002

Leave Link 502 at Tue Sep 17 14:42:23 2019, MaxMem= 2415919104 cpu: 1458.4

(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= 15325 LenP2D= 41264.

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 = 244

Leave Link 701 at Tue Sep 17 14:42:27 2019, MaxMem= 2415919104 cpu: 69.0

(Enter /home/blab/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Tue Sep 17 14:42:27 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 14:42:37 2019, MaxMem= 2415919104 cpu: 176.5

(Enter /home/blab/g09/l716.exe)

Dipole =-4.24549285D-13 7.54951657D-15-6.66133815D-16

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000008327 0.000002651 -0.000000000

2 7 -0.000136026 -0.000444381 0.000000000

3 6 0.000006118 0.000025925 -0.000000000

4 6 -0.000017419 -0.000005051 0.000000000

5 6 0.000004324 0.000016305 0.000000000

6 7 -0.000030173 -0.000030322 0.000000000

7 6 0.000005502 0.000015439 0.000000000

8 7 0.000477451 -0.000197312 -0.000000000

9 6 -0.000001594 0.000018433 -0.000000000

10 6 0.000009313 -0.000030205 0.000000000

11 6 -0.000011913 0.000018359 -0.000000000

12 7 -0.000004073 -0.000000384 0.000000000

13 6 -0.000009313 0.000030205 -0.000000000

14 6 0.000011913 -0.000018359 -0.000000000

15 6 -0.000005502 -0.000015439 -0.000000000

16 7 -0.000477451 0.000197312 0.000000000

17 6 0.000001594 -0.000018433 0.000000000

18 7 0.000030173 0.000030322 -0.000000000

19 7 0.000136026 0.000444381 -0.000000000

20 6 -0.000006118 -0.000025925 0.000000000

21 6 0.000017419 0.000005051 0.000000000

22 6 -0.000004324 -0.000016305 0.000000000

23 6 -0.000008327 -0.000002651 0.000000000

24 7 0.000004073 0.000000384 0.000000000

25 30 0.000000000 0.000000000 0.000000000

26 6 0.000019024 0.000013802 0.000000000

27 1 -0.000005548 -0.000013466 -0.000000000

28 6 -0.000029322 0.000009957 -0.000000000

29 1 0.000018036 -0.000006468 0.000000000

30 6 0.000029322 -0.000009957 -0.000000000

31 1 -0.000018036 0.000006468 -0.000000000

32 6 -0.000019024 -0.000013802 0.000000000

33 1 0.000005548 0.000013466 0.000000000

34 1 -0.000009634 0.000011125 0.000000000

35 1 0.000005970 -0.000003564 0.000001885

36 1 0.000005970 -0.000003564 -0.000001885

37 1 0.000011467 0.000004701 0.000000076

38 1 0.000011467 0.000004701 -0.000000076

39 1 -0.000010972 -0.000008609 0.000000000

40 1 -0.000011467 -0.000004701 0.000000076

41 1 -0.000011467 -0.000004701 -0.000000076

42 1 0.000010972 0.000008609 -0.000000000

43 1 -0.000005970 0.000003564 0.000001885

44 1 -0.000005970 0.000003564 -0.000001885

45 1 0.000009634 -0.000011125 -0.000000000

-------------------------------------------------------------------

Cartesian Forces: Max 0.000477451 RMS 0.000085298

Leave Link 716 at Tue Sep 17 14:42:37 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 0.000357951 RMS 0.000047728

Search for a local minimum.

Step number 31 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 12 13 14 15

16 17 18 19 20

21 22 23 24 25

26 27 28 29 30

31

DE= -9.98D-05 DEPred=-9.93D-05 R= 1.00D+00

TightC=F SS= 1.41D+00 RLast= 3.61D-02 DXNew= 8.4090D-02 1.0843D-01

Trust test= 1.00D+00 RLast= 3.61D-02 DXMaxT set to 8.41D-02

ITU= 1 -1 -1 1 1 -1 1 -1 -1 1 0 0 1 -1 -1 1 1 -1 1 1

ITU= 1 -1 0 1 -1 1 1 1 1 0 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01337

Eigenvalues --- 0.01338 0.01346 0.01347 0.01604 0.01623

Eigenvalues --- 0.01631 0.01640 0.01774 0.01793 0.01809

Eigenvalues --- 0.01823 0.01890 0.01909 0.01939 0.01950

Eigenvalues --- 0.01997 0.02000 0.02045 0.02047 0.02070

Eigenvalues --- 0.02087 0.02103 0.02110 0.02115 0.02205

Eigenvalues --- 0.02312 0.02316 0.02351 0.02372 0.06527

Eigenvalues --- 0.07152 0.07195 0.07195 0.07198 0.07198

Eigenvalues --- 0.07313 0.07393 0.07953 0.08186 0.11507

Eigenvalues --- 0.13086 0.14001 0.14498 0.14500 0.15028

Eigenvalues --- 0.15333 0.15951 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16141 0.16400 0.17258

Eigenvalues --- 0.20668 0.20872 0.22060 0.22092 0.22616

Eigenvalues --- 0.23841 0.23854 0.23862 0.24814 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25527 0.26788 0.28078 0.29787 0.31157

Eigenvalues --- 0.31562 0.33049 0.33189 0.33197 0.33282

Eigenvalues --- 0.33282 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33724 0.33727 0.33912 0.34374

Eigenvalues --- 0.34428 0.34437 0.34437 0.34556 0.35555

Eigenvalues --- 0.35564 0.35637 0.35682 0.35682 0.35743

Eigenvalues --- 0.37205 0.38549 0.41638 0.41817 0.42279

Eigenvalues --- 0.45926 0.47134 0.48966 0.48981 0.50075

Eigenvalues --- 0.51358 0.51361 0.52988 0.53308 0.54019

Eigenvalues --- 0.54026 0.55889 0.56320 0.56328

DIIS coeff's: 0.95054 0.03763 -0.16481 0.02696 0.16053

DIIS coeff's: 0.04982 -0.00233 -0.00430 -0.00041 -0.00160

DIIS coeff's: -0.02056 0.00706 0.00971 -0.00085 0.13493

DIIS coeff's: -0.07885 -0.13593 0.02418 0.00015 -0.00220

DIIS coeff's: 0.00833 -0.00353 0.00055 0.00976 -0.00456

DIIS coeff's: -0.01328 0.02069 -0.02174 0.01595 -0.00171

DIIS coeff's: -0.00008

Cosine: 0.773 > 0.500

Length: 0.145

GDIIS step was calculated using 31 of the last 31 vectors.

Iteration 1 RMS(Cart)= 0.00009533 RMS(Int)= 0.00000028

Iteration 2 RMS(Cart)= 0.00000001 RMS(Int)= 0.00000028

ITry= 1 IFail=0 DXMaxC= 3.86D-04 DCOld= 1.00D+10 DXMaxT= 8.41D-02 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 8.88D-11 for atom 41.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58169 -0.00001 0.00007 -0.00000 0.00007 2.58176

R2 2.73239 0.00001 0.00005 -0.00000 0.00005 2.73244

R3 2.58665 0.00010 -0.00010 -0.00000 -0.00010 2.58655

R4 2.56256 -0.00004 -0.00013 -0.00000 -0.00013 2.56243

R5 3.79786 0.00030 0.00027 0.00000 0.00027 3.79812

R6 2.77350 -0.00000 0.00014 0.00000 0.00014 2.77365

R7 2.57978 0.00007 -0.00004 0.00000 -0.00004 2.57974

R8 2.59786 0.00004 -0.00004 -0.00000 -0.00004 2.59783

R9 2.81328 -0.00001 -0.00002 -0.00000 -0.00002 2.81326

R10 2.04304 0.00001 0.00001 0.00000 0.00001 2.04304

R11 2.49711 0.00010 0.00017 -0.00000 0.00017 2.49728

R12 2.58321 -0.00002 -0.00015 0.00000 -0.00015 2.58306

R13 2.80020 0.00001 -0.00000 -0.00000 -0.00000 2.80019

R14 2.57787 -0.00002 0.00006 0.00000 0.00006 2.57792

R15 3.78111 0.00036 0.00038 -0.00000 0.00038 3.78149

R16 2.84078 0.00002 -0.00008 0.00000 -0.00008 2.84070

R17 2.48791 0.00009 0.00006 0.00000 0.00006 2.48798

R18 2.55012 0.00003 0.00006 -0.00000 0.00006 2.55018

R19 2.80698 -0.00001 0.00001 0.00000 0.00001 2.80699

R20 2.04321 0.00001 0.00001 0.00000 0.00001 2.04322

R21 2.48791 0.00009 0.00006 0.00000 0.00006 2.48798

R22 2.55012 0.00003 0.00006 -0.00000 0.00006 2.55018

R23 2.84078 0.00002 -0.00008 0.00000 -0.00008 2.84070

R24 2.80698 -0.00001 0.00001 0.00000 0.00001 2.80699

R25 2.80020 0.00001 -0.00000 -0.00000 -0.00000 2.80019

R26 2.04321 0.00001 0.00001 0.00000 0.00001 2.04322

R27 2.58321 -0.00002 -0.00015 0.00000 -0.00015 2.58306

R28 2.49711 0.00010 0.00017 -0.00000 0.00017 2.49728

R29 2.57787 -0.00002 0.00006 0.00000 0.00006 2.57792

R30 3.78111 0.00036 0.00038 -0.00000 0.00038 3.78149

R31 2.57978 0.00007 -0.00004 0.00000 -0.00004 2.57974

R32 2.56256 -0.00004 -0.00013 -0.00000 -0.00013 2.56243

R33 2.58169 -0.00001 0.00007 -0.00000 0.00007 2.58176

R34 3.79786 0.00030 0.00027 0.00000 0.00027 3.79812

R35 2.77350 -0.00000 0.00014 0.00000 0.00014 2.77365

R36 2.59786 0.00004 -0.00004 -0.00000 -0.00004 2.59783

R37 2.81328 -0.00001 -0.00002 -0.00000 -0.00002 2.81326

R38 2.73239 0.00001 0.00005 -0.00000 0.00005 2.73244

R39 2.04304 0.00001 0.00001 0.00000 0.00001 2.04304

R40 2.58665 0.00010 -0.00010 -0.00000 -0.00010 2.58655

R41 2.06237 0.00000 0.00000 -0.00000 0.00000 2.06237

R42 2.06951 0.00001 0.00000 -0.00000 0.00000 2.06952

R43 2.06951 0.00001 0.00000 -0.00000 0.00000 2.06952

R44 2.06875 0.00000 0.00000 -0.00000 0.00000 2.06875

R45 2.06875 0.00000 0.00000 -0.00000 0.00000 2.06875

R46 2.06158 0.00000 0.00000 0.00000 0.00000 2.06159

R47 2.06875 0.00000 0.00000 -0.00000 0.00000 2.06875

R48 2.06875 0.00000 0.00000 -0.00000 0.00000 2.06875

R49 2.06158 0.00000 0.00000 0.00000 0.00000 2.06159

R50 2.06951 0.00001 0.00000 -0.00000 0.00000 2.06952

R51 2.06951 0.00001 0.00000 -0.00000 0.00000 2.06952

R52 2.06237 0.00000 0.00000 -0.00000 0.00000 2.06237

A1 1.89244 -0.00006 -0.00009 -0.00000 -0.00009 1.89235

A2 2.20477 0.00002 0.00002 -0.00000 0.00002 2.20479

A3 2.18597 0.00004 0.00007 0.00000 0.00007 2.18605

A4 1.90686 0.00009 0.00013 0.00000 0.00013 1.90698

A5 2.19229 -0.00005 -0.00010 0.00000 -0.00010 2.19219

A6 2.18403 -0.00003 -0.00002 -0.00000 -0.00002 2.18401

A7 1.89531 -0.00005 -0.00008 -0.00000 -0.00008 1.89523

A8 2.22366 0.00002 0.00008 0.00000 0.00008 2.22374

A9 2.16421 0.00003 0.00001 -0.00000 0.00001 2.16422

A10 1.85188 0.00002 0.00003 -0.00000 0.00003 1.85191

A11 2.17349 -0.00002 -0.00005 0.00000 -0.00005 2.17344

A12 2.25781 0.00001 0.00003 -0.00000 0.00003 2.25784

A13 1.87828 0.00000 0.00002 0.00000 0.00002 1.87830

A14 2.18093 0.00001 0.00002 -0.00000 0.00002 2.18095

A15 2.22397 -0.00001 -0.00004 -0.00000 -0.00004 2.22393

A16 2.16822 0.00006 0.00002 -0.00000 0.00002 2.16825

A17 2.23116 0.00000 -0.00000 -0.00000 -0.00000 2.23116

A18 2.16833 0.00005 0.00007 0.00000 0.00007 2.16839

A19 1.88369 -0.00006 -0.00006 0.00000 -0.00006 1.88363

A20 1.91410 0.00010 0.00012 -0.00000 0.00012 1.91423

A21 2.18901 -0.00005 -0.00002 0.00000 -0.00002 2.18900

A22 2.18007 -0.00005 -0.00011 -0.00000 -0.00011 2.17996

A23 1.88453 -0.00007 -0.00009 -0.00000 -0.00009 1.88444

A24 2.24684 0.00000 -0.00004 0.00000 -0.00004 2.24680

A25 2.15182 0.00006 0.00013 0.00000 0.00013 2.15194

A26 1.85654 0.00002 0.00002 -0.00000 0.00002 1.85655

A27 2.15441 0.00000 0.00005 0.00000 0.00005 2.15446

A28 2.27224 -0.00002 -0.00007 0.00000 -0.00007 2.27217

A29 1.88591 0.00001 0.00001 0.00000 0.00001 1.88592

A30 2.16471 0.00001 0.00006 -0.00000 0.00006 2.16477

A31 2.23256 -0.00002 -0.00007 -0.00000 -0.00007 2.23250

A32 2.17108 0.00008 0.00018 0.00000 0.00018 2.17126

A33 1.85654 0.00002 0.00002 -0.00000 0.00002 1.85655

A34 2.27224 -0.00002 -0.00007 0.00000 -0.00007 2.27217

A35 2.15441 0.00000 0.00005 0.00000 0.00005 2.15446

A36 1.88591 0.00001 0.00001 0.00000 0.00001 1.88592

A37 2.23256 -0.00002 -0.00007 -0.00000 -0.00007 2.23250

A38 2.16471 0.00001 0.00006 -0.00000 0.00006 2.16477

A39 1.88369 -0.00006 -0.00006 0.00000 -0.00006 1.88363

A40 2.16833 0.00005 0.00007 0.00000 0.00007 2.16839

A41 2.23116 0.00000 -0.00000 -0.00000 -0.00000 2.23116

A42 1.91410 0.00010 0.00012 -0.00000 0.00012 1.91423

A43 2.18901 -0.00005 -0.00002 0.00000 -0.00002 2.18900

A44 2.18007 -0.00005 -0.00011 -0.00000 -0.00011 2.17996

A45 2.15182 0.00006 0.00013 0.00000 0.00013 2.15194

A46 2.24684 0.00000 -0.00004 0.00000 -0.00004 2.24680

A47 1.88453 -0.00007 -0.00009 -0.00000 -0.00009 1.88444

A48 2.16822 0.00006 0.00002 -0.00000 0.00002 2.16825

A49 1.90686 0.00009 0.00013 0.00000 0.00013 1.90698

A50 2.18403 -0.00003 -0.00002 -0.00000 -0.00002 2.18401

A51 2.19229 -0.00005 -0.00010 0.00000 -0.00010 2.19219

A52 2.22366 0.00002 0.00008 0.00000 0.00008 2.22374

A53 2.16421 0.00003 0.00001 -0.00000 0.00001 2.16422

A54 1.89531 -0.00005 -0.00008 -0.00000 -0.00008 1.89523

A55 1.85188 0.00002 0.00003 -0.00000 0.00003 1.85191

A56 2.17349 -0.00002 -0.00005 0.00000 -0.00005 2.17344

A57 2.25781 0.00001 0.00003 -0.00000 0.00003 2.25784

A58 1.87828 0.00000 0.00002 0.00000 0.00002 1.87830

A59 2.22397 -0.00001 -0.00004 -0.00000 -0.00004 2.22393

A60 2.18093 0.00001 0.00002 -0.00000 0.00002 2.18095

A61 1.89244 -0.00006 -0.00009 -0.00000 -0.00009 1.89235

A62 2.20477 0.00002 0.00002 -0.00000 0.00002 2.20479

A63 2.18597 0.00004 0.00007 0.00000 0.00007 2.18605

A64 2.17108 0.00008 0.00018 0.00000 0.00018 2.17126

A65 1.57028 -0.00001 -0.00005 0.00000 -0.00005 1.57022

A66 1.57132 0.00001 0.00005 -0.00000 0.00005 1.57137

A67 1.57132 0.00001 0.00005 -0.00000 0.00005 1.57137

A68 1.57028 -0.00001 -0.00005 0.00000 -0.00005 1.57022

A69 1.94307 -0.00002 -0.00001 -0.00000 -0.00002 1.94306

A70 1.94056 0.00001 0.00000 -0.00000 0.00000 1.94056

A71 1.94056 0.00001 0.00000 -0.00000 0.00000 1.94056

A72 1.88947 0.00001 0.00001 0.00000 0.00001 1.88948

A73 1.88947 0.00001 0.00001 0.00000 0.00001 1.88948

A74 1.85754 -0.00000 -0.00001 0.00000 -0.00001 1.85753

A75 1.93382 0.00002 0.00004 0.00000 0.00004 1.93385

A76 1.93382 0.00002 0.00004 0.00000 0.00004 1.93385

A77 1.94530 -0.00003 -0.00004 -0.00000 -0.00004 1.94526

A78 1.85778 -0.00001 -0.00000 0.00000 -0.00000 1.85777

A79 1.89520 0.00000 -0.00002 0.00000 -0.00002 1.89519

A80 1.89520 0.00000 -0.00002 0.00000 -0.00002 1.89519

A81 1.93382 0.00002 0.00004 0.00000 0.00004 1.93385

A82 1.93382 0.00002 0.00004 0.00000 0.00004 1.93385

A83 1.94530 -0.00003 -0.00004 -0.00000 -0.00004 1.94526

A84 1.85778 -0.00001 -0.00000 0.00000 -0.00000 1.85777

A85 1.89520 0.00000 -0.00002 0.00000 -0.00002 1.89519

A86 1.89520 0.00000 -0.00002 0.00000 -0.00002 1.89519

A87 1.94056 0.00001 0.00000 -0.00000 0.00000 1.94056

A88 1.94056 0.00001 0.00000 -0.00000 0.00000 1.94056

A89 1.94307 -0.00002 -0.00001 -0.00000 -0.00002 1.94306

A90 1.85754 -0.00000 -0.00001 0.00000 -0.00001 1.85753

A91 1.88947 0.00001 0.00001 0.00000 0.00001 1.88948

A92 1.88947 0.00001 0.00001 0.00000 0.00001 1.88948

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 1.03319 0.00000 -0.00001 0.00000 -0.00001 1.03319

D31 -1.03319 -0.00000 0.00001 -0.00000 0.00001 -1.03319

D32 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.10840 0.00000 -0.00001 0.00000 -0.00001 -2.10841

D34 2.10840 -0.00000 0.00001 -0.00000 0.00001 2.10841

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 1.02902 0.00000 0.00002 0.00000 0.00002 1.02904

D64 -1.02902 -0.00000 -0.00002 -0.00000 -0.00002 -1.02904

D65 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D66 -2.11257 0.00000 0.00002 0.00000 0.00002 -2.11255

D67 2.11257 -0.00000 -0.00002 -0.00000 -0.00002 2.11255

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 -2.11257 0.00000 0.00002 0.00000 0.00002 -2.11255

D80 2.11257 -0.00000 -0.00002 -0.00000 -0.00002 2.11255

D81 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D82 1.02902 0.00000 0.00002 0.00000 0.00002 1.02904

D83 -1.02902 -0.00000 -0.00002 -0.00000 -0.00002 -1.02904

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 1.03319 0.00000 -0.00001 0.00000 -0.00001 1.03319

D126 -1.03319 -0.00000 0.00001 -0.00000 0.00001 -1.03319

D127 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D128 -2.10840 0.00000 -0.00001 0.00000 -0.00001 -2.10841

D129 2.10840 -0.00000 0.00001 -0.00000 0.00001 2.10841

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 0.000358 0.000450 YES

RMS Force 0.000048 0.000300 YES

Maximum Displacement 0.000386 0.001800 YES

RMS Displacement 0.000095 0.001200 YES

Predicted change in Energy=-5.989161D-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 = 0.0 !

! R2 R(1,5) 1.4459 -DE/DX = 0.0 !

! R3 R(1,12) 1.3688 -DE/DX = 0.0001 !

! R4 R(2,3) 1.3561 -DE/DX = 0.0 !

! R5 R(2,25) 2.0097 -DE/DX = 0.0003 !

! R6 R(3,4) 1.4677 -DE/DX = 0.0 !

! R7 R(3,6) 1.3652 -DE/DX = 0.0001 !

! R8 R(4,5) 1.3747 -DE/DX = 0.0 !

! R9 R(4,26) 1.4887 -DE/DX = 0.0 !

! R10 R(5,27) 1.0811 -DE/DX = 0.0 !

! R11 R(6,7) 1.3214 -DE/DX = 0.0001 !

! R12 R(7,8) 1.367 -DE/DX = 0.0 !

! R13 R(7,11) 1.4818 -DE/DX = 0.0 !

! R14 R(8,9) 1.3641 -DE/DX = 0.0 !

! R15 R(8,25) 2.0009 -DE/DX = 0.0004 !

! R16 R(9,10) 1.5033 -DE/DX = 0.0 !

! R17 R(9,24) 1.3165 -DE/DX = 0.0001 !

! R18 R(10,11) 1.3495 -DE/DX = 0.0 !

! R19 R(10,28) 1.4854 -DE/DX = 0.0 !

! R20 R(11,29) 1.0812 -DE/DX = 0.0 !

! R21 R(12,17) 1.3165 -DE/DX = 0.0001 !

! R22 R(13,14) 1.3495 -DE/DX = 0.0 !

! R23 R(13,17) 1.5033 -DE/DX = 0.0 !

! R24 R(13,30) 1.4854 -DE/DX = 0.0 !

! R25 R(14,15) 1.4818 -DE/DX = 0.0 !

! R26 R(14,31) 1.0812 -DE/DX = 0.0 !

! R27 R(15,16) 1.367 -DE/DX = 0.0 !

! R28 R(15,18) 1.3214 -DE/DX = 0.0001 !

! R29 R(16,17) 1.3641 -DE/DX = 0.0 !

! R30 R(16,25) 2.0009 -DE/DX = 0.0004 !

! R31 R(18,20) 1.3652 -DE/DX = 0.0001 !

! R32 R(19,20) 1.3561 -DE/DX = 0.0 !

! R33 R(19,23) 1.3662 -DE/DX = 0.0 !

! R34 R(19,25) 2.0097 -DE/DX = 0.0003 !

! R35 R(20,21) 1.4677 -DE/DX = 0.0 !

! R36 R(21,22) 1.3747 -DE/DX = 0.0 !

! R37 R(21,32) 1.4887 -DE/DX = 0.0 !

! R38 R(22,23) 1.4459 -DE/DX = 0.0 !

! R39 R(22,33) 1.0811 -DE/DX = 0.0 !

! R40 R(23,24) 1.3688 -DE/DX = 0.0001 !

! R41 R(26,34) 1.0914 -DE/DX = 0.0 !

! R42 R(26,35) 1.0951 -DE/DX = 0.0 !

! R43 R(26,36) 1.0951 -DE/DX = 0.0 !

! R44 R(28,37) 1.0947 -DE/DX = 0.0 !

! R45 R(28,38) 1.0947 -DE/DX = 0.0 !

! R46 R(28,39) 1.0909 -DE/DX = 0.0 !

! R47 R(30,40) 1.0947 -DE/DX = 0.0 !

! R48 R(30,41) 1.0947 -DE/DX = 0.0 !

! R49 R(30,42) 1.0909 -DE/DX = 0.0 !

! R50 R(32,43) 1.0951 -DE/DX = 0.0 !

! R51 R(32,44) 1.0951 -DE/DX = 0.0 !

! R52 R(32,45) 1.0914 -DE/DX = 0.0 !

! A1 A(2,1,5) 108.429 -DE/DX = -0.0001 !

! A2 A(2,1,12) 126.3239 -DE/DX = 0.0 !

! A3 A(5,1,12) 125.2471 -DE/DX = 0.0 !

! A4 A(1,2,3) 109.2549 -DE/DX = 0.0001 !

! A5 A(1,2,25) 125.6092 -DE/DX = -0.0001 !

! A6 A(3,2,25) 125.1359 -DE/DX = 0.0 !

! A7 A(2,3,4) 108.5934 -DE/DX = -0.0001 !

! A8 A(2,3,6) 127.4065 -DE/DX = 0.0 !

! A9 A(4,3,6) 124.0002 -DE/DX = 0.0 !

! A10 A(3,4,5) 106.1051 -DE/DX = 0.0 !

! A11 A(3,4,26) 124.5318 -DE/DX = 0.0 !

! A12 A(5,4,26) 129.3631 -DE/DX = 0.0 !

! A13 A(1,5,4) 107.6177 -DE/DX = 0.0 !

! A14 A(1,5,27) 124.9583 -DE/DX = 0.0 !

! A15 A(4,5,27) 127.4241 -DE/DX = 0.0 !

! A16 A(3,6,7) 124.2301 -DE/DX = 0.0001 !

! A17 A(6,7,8) 127.8362 -DE/DX = 0.0 !

! A18 A(6,7,11) 124.236 -DE/DX = 0.0001 !

! A19 A(8,7,11) 107.9277 -DE/DX = -0.0001 !

! A20 A(7,8,9) 109.6701 -DE/DX = 0.0001 !

! A21 A(7,8,25) 125.4211 -DE/DX = 0.0 !

! A22 A(9,8,25) 124.9088 -DE/DX = -0.0001 !

! A23 A(8,9,10) 107.9756 -DE/DX = -0.0001 !

! A24 A(8,9,24) 128.7344 -DE/DX = 0.0 !

! A25 A(10,9,24) 123.29 -DE/DX = 0.0001 !

! A26 A(9,10,11) 106.3719 -DE/DX = 0.0 !

! A27 A(9,10,28) 123.4386 -DE/DX = 0.0 !

! A28 A(11,10,28) 130.1895 -DE/DX = 0.0 !

! A29 A(7,11,10) 108.0546 -DE/DX = 0.0 !

! A30 A(7,11,29) 124.0288 -DE/DX = 0.0 !

! A31 A(10,11,29) 127.9165 -DE/DX = 0.0 !

! A32 A(1,12,17) 124.3939 -DE/DX = 0.0001 !

! A33 A(14,13,17) 106.3719 -DE/DX = 0.0 !

! A34 A(14,13,30) 130.1895 -DE/DX = 0.0 !

! A35 A(17,13,30) 123.4386 -DE/DX = 0.0 !

! A36 A(13,14,15) 108.0546 -DE/DX = 0.0 !

! A37 A(13,14,31) 127.9165 -DE/DX = 0.0 !

! A38 A(15,14,31) 124.0288 -DE/DX = 0.0 !

! A39 A(14,15,16) 107.9277 -DE/DX = -0.0001 !

! A40 A(14,15,18) 124.236 -DE/DX = 0.0001 !

! A41 A(16,15,18) 127.8362 -DE/DX = 0.0 !

! A42 A(15,16,17) 109.6701 -DE/DX = 0.0001 !

! A43 A(15,16,25) 125.4211 -DE/DX = 0.0 !

! A44 A(17,16,25) 124.9088 -DE/DX = -0.0001 !

! A45 A(12,17,13) 123.29 -DE/DX = 0.0001 !

! A46 A(12,17,16) 128.7344 -DE/DX = 0.0 !

! A47 A(13,17,16) 107.9756 -DE/DX = -0.0001 !

! A48 A(15,18,20) 124.2301 -DE/DX = 0.0001 !

! A49 A(20,19,23) 109.2549 -DE/DX = 0.0001 !

! A50 A(20,19,25) 125.1359 -DE/DX = 0.0 !

! A51 A(23,19,25) 125.6092 -DE/DX = -0.0001 !

! A52 A(18,20,19) 127.4065 -DE/DX = 0.0 !

! A53 A(18,20,21) 124.0002 -DE/DX = 0.0 !

! A54 A(19,20,21) 108.5934 -DE/DX = -0.0001 !

! A55 A(20,21,22) 106.1051 -DE/DX = 0.0 !

! A56 A(20,21,32) 124.5318 -DE/DX = 0.0 !

! A57 A(22,21,32) 129.3631 -DE/DX = 0.0 !

! A58 A(21,22,23) 107.6177 -DE/DX = 0.0 !

! A59 A(21,22,33) 127.4241 -DE/DX = 0.0 !

! A60 A(23,22,33) 124.9583 -DE/DX = 0.0 !

! A61 A(19,23,22) 108.429 -DE/DX = -0.0001 !

! A62 A(19,23,24) 126.3239 -DE/DX = 0.0 !

! A63 A(22,23,24) 125.2471 -DE/DX = 0.0 !

! A64 A(9,24,23) 124.3939 -DE/DX = 0.0001 !

! A65 A(2,25,8) 89.9702 -DE/DX = 0.0 !

! A66 A(2,25,16) 90.0298 -DE/DX = 0.0 !

! A67 A(8,25,19) 90.0298 -DE/DX = 0.0 !

! A68 A(16,25,19) 89.9702 -DE/DX = 0.0 !

! A69 A(4,26,34) 111.33 -DE/DX = 0.0 !

! A70 A(4,26,35) 111.186 -DE/DX = 0.0 !

! A71 A(4,26,36) 111.186 -DE/DX = 0.0 !

! A72 A(34,26,35) 108.2588 -DE/DX = 0.0 !

! A73 A(34,26,36) 108.2588 -DE/DX = 0.0 !

! A74 A(35,26,36) 106.4292 -DE/DX = 0.0 !

! A75 A(10,28,37) 110.7995 -DE/DX = 0.0 !

! A76 A(10,28,38) 110.7995 -DE/DX = 0.0 !

! A77 A(10,28,39) 111.4574 -DE/DX = 0.0 !

! A78 A(37,28,38) 106.4428 -DE/DX = 0.0 !

! A79 A(37,28,39) 108.587 -DE/DX = 0.0 !

! A80 A(38,28,39) 108.587 -DE/DX = 0.0 !

! A81 A(13,30,40) 110.7995 -DE/DX = 0.0 !

! A82 A(13,30,41) 110.7995 -DE/DX = 0.0 !

! A83 A(13,30,42) 111.4574 -DE/DX = 0.0 !

! A84 A(40,30,41) 106.4428 -DE/DX = 0.0 !

! A85 A(40,30,42) 108.587 -DE/DX = 0.0 !

! A86 A(41,30,42) 108.587 -DE/DX = 0.0 !

! A87 A(21,32,43) 111.186 -DE/DX = 0.0 !

! A88 A(21,32,44) 111.186 -DE/DX = 0.0 !

! A89 A(21,32,45) 111.33 -DE/DX = 0.0 !

! A90 A(43,32,44) 106.4292 -DE/DX = 0.0 !

! A91 A(43,32,45) 108.2588 -DE/DX = 0.0 !

! A92 A(44,32,45) 108.2588 -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) 59.1975 -DE/DX = 0.0 !

! D31 D(3,4,26,36) -59.1975 -DE/DX = 0.0 !

! D32 D(5,4,26,34) 0.0 -DE/DX = 0.0 !

! D33 D(5,4,26,35) -120.8025 -DE/DX = 0.0 !

! D34 D(5,4,26,36) 120.8025 -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) 58.9584 -DE/DX = 0.0 !

! D64 D(9,10,28,38) -58.9584 -DE/DX = 0.0 !

! D65 D(9,10,28,39) 180.0 -DE/DX = 0.0 !

! D66 D(11,10,28,37) -121.0416 -DE/DX = 0.0 !

! D67 D(11,10,28,38) 121.0416 -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) -121.0416 -DE/DX = 0.0 !

! D80 D(14,13,30,41) 121.0416 -DE/DX = 0.0 !

! D81 D(14,13,30,42) 0.0 -DE/DX = 0.0 !

! D82 D(17,13,30,40) 58.9584 -DE/DX = 0.0 !

! D83 D(17,13,30,41) -58.9584 -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) 59.1975 -DE/DX = 0.0 !

! D126 D(20,21,32,44) -59.1975 -DE/DX = 0.0 !

! D127 D(20,21,32,45) 180.0 -DE/DX = 0.0 !

! D128 D(22,21,32,43) -120.8025 -DE/DX = 0.0 !

! D129 D(22,21,32,44) 120.8025 -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 42 12.569 Angstoms.

Leave Link 103 at Tue Sep 17 14:42:37 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 -2.073315 -2.191841 0.000000

2 7 0 -0.746589 -1.865919 0.000000

3 6 0 -0.006905 -3.002466 0.000000

4 6 0 -0.917541 -4.153471 0.000000

5 6 0 -2.189957 -3.633049 0.000000

6 7 0 1.354326 -3.106004 0.000000

7 6 0 2.178365 -2.073000 0.000000

8 7 0 1.857303 -0.744263 0.000000

9 6 0 2.998067 0.003772 0.000000

10 6 0 4.170114 -0.937577 0.000000

11 6 0 3.655909 -2.185232 0.000000

12 7 0 -3.123801 -1.314302 0.000000

13 6 0 -4.170114 0.937577 0.000000

14 6 0 -3.655909 2.185232 0.000000

15 6 0 -2.178365 2.073000 0.000000

16 7 0 -1.857303 0.744263 0.000000

17 6 0 -2.998067 -0.003772 0.000000

18 7 0 -1.354326 3.106004 0.000000

19 7 0 0.746589 1.865919 0.000000

20 6 0 0.006905 3.002466 0.000000

21 6 0 0.917541 4.153471 0.000000

22 6 0 2.189957 3.633049 0.000000

23 6 0 2.073315 2.191841 0.000000

24 7 0 3.123801 1.314302 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.479341 -5.576242 0.000000

27 1 0 -3.123102 -4.179016 0.000000

28 6 0 5.584470 -0.483720 0.000000

29 1 0 4.191364 -3.124554 0.000000

30 6 0 -5.584470 0.483720 0.000000

31 1 0 -4.191364 3.124554 0.000000

32 6 0 0.479341 5.576242 0.000000

33 1 0 3.123102 4.179016 0.000000

34 1 0 -1.334061 -6.254859 0.000000

35 1 0 0.136886 -5.800576 0.877080

36 1 0 0.136886 -5.800576 -0.877080

37 1 0 5.793373 0.137541 0.876832

38 1 0 5.793373 0.137541 -0.876832

39 1 0 6.274693 -1.328556 0.000000

40 1 0 -5.793373 -0.137541 0.876832

41 1 0 -5.793373 -0.137541 -0.876832

42 1 0 -6.274693 1.328556 0.000000

43 1 0 -0.136886 5.800576 0.877080

44 1 0 -0.136886 5.800576 -0.877080

45 1 0 1.334061 6.254859 0.000000

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Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.366172 0.000000

3 C 2.219721 1.356050 0.000000

4 C 2.276797 2.293931 1.467676 0.000000

5 C 1.445920 2.281679 2.272301 1.374729 0.000000

6 N 3.547452 2.439601 1.365162 2.501713 3.583255

7 C 4.253341 2.932276 2.374724 3.730013 4.638533

8 N 4.188704 2.835202 2.928268 4.395732 4.972464

9 C 5.526267 4.185474 4.250567 5.710924 6.335776

10 C 6.368170 5.003578 4.659534 6.018822 6.907682

11 C 5.729227 4.414063 3.752875 4.978997 6.022484

12 N 1.368794 2.440372 3.544706 3.595617 2.499730

13 C 3.766939 4.424943 5.732038 6.041358 4.981129

14 C 4.654393 4.987581 6.342511 6.904913 6.000117

15 C 4.266135 4.191070 5.520471 6.352844 5.706061

16 N 2.944039 2.836677 4.178750 4.987078 4.389933

17 C 2.375460 2.921770 4.235471 4.642046 3.718157

18 N 5.346411 5.008928 6.255314 7.272603 6.790664

19 N 4.941384 4.019478 4.926350 6.245189 6.233936

20 C 5.595367 4.926350 6.004948 7.215403 6.989725

21 C 7.014856 6.245189 7.215403 8.507221 8.383701

22 C 7.218367 6.233936 6.989725 8.383701 8.484092

23 C 6.034170 4.941384 5.595367 7.014856 7.218367

24 N 6.269215 5.009364 5.332524 6.799191 7.260324

25 Zn 3.017085 2.009739 3.002474 4.253611 4.242046

26 C 3.740979 3.719935 2.616776 1.488723 2.588862

27 H 2.247425 3.316358 3.330909 2.205708 1.081129

28 C 7.845976 6.480184 6.132499 7.466138 8.388086

29 H 6.333732 5.095836 4.200044 5.211486 6.401549

30 C 4.414390 5.378279 6.577440 6.579040 5.335776

31 H 5.722778 6.063934 7.419574 7.980449 7.047753

32 C 8.176745 7.542457 8.592477 9.829475 9.588336

33 H 8.221348 7.177448 7.833941 9.260515 9.447590

34 H 4.129723 4.428083 3.512749 2.142270 2.757979

35 H 4.321716 4.126902 2.935876 2.143371 3.298734

36 H 4.321716 4.126902 2.935876 2.143371 3.298734

37 H 8.251038 6.895926 6.653698 8.013613 8.872415

38 H 8.251038 6.895926 6.653698 8.013613 8.872415

39 H 8.392526 7.041815 6.500803 7.727120 8.772741

40 H 4.339103 5.406122 6.516122 6.377324 5.096275

41 H 4.339103 5.406122 6.516122 6.377324 5.096275

42 H 5.481311 6.384716 7.618590 7.664965 6.426709

43 H 8.270294 7.740553 8.847582 10.023061 9.694207

44 H 8.270294 7.740553 8.847582 10.023061 9.694207

45 H 9.108070 8.383087 9.353943 10.649086 10.497115

6 7 8 9 10

6 N 0.000000

7 C 1.321415 0.000000

8 N 2.414707 1.366977 0.000000

9 C 3.517470 2.232688 1.364147 0.000000

10 C 3.553975 2.292651 2.320876 1.503275 0.000000

11 C 2.478932 1.481800 2.304642 2.285716 1.349463

12 N 4.823258 5.356173 5.013616 6.262155 7.303638

13 C 6.846166 7.026149 6.257663 7.228749 8.548428

14 C 7.286949 7.222970 6.243192 7.002440 8.426066

15 C 6.269130 6.014185 4.921747 5.574689 7.026149

16 N 5.013892 4.921747 4.001750 4.911511 6.257663

17 C 5.344826 5.574689 4.911511 5.996139 7.228749

18 N 6.776860 6.269130 5.013892 5.344826 6.846166

19 N 5.008928 4.191070 2.836677 2.921770 4.424943

20 C 6.255314 5.520471 4.178750 4.235471 5.732038

21 C 7.272603 6.352844 4.987078 4.642046 6.041358

22 C 6.790664 5.706061 4.389933 3.718157 4.981129

23 C 5.346411 4.266135 2.944039 2.375460 3.766939

24 N 4.761318 3.516769 2.416962 1.316548 2.483089

25 Zn 3.388430 3.007093 2.000875 2.998069 4.274214

26 C 3.076428 4.397284 5.367302 6.574870 6.567697

27 H 4.604206 5.704459 6.049956 7.413800 7.981098

28 C 4.976996 3.758638 3.736262 2.631944 1.485391

29 H 2.837099 2.271108 3.333711 3.348191 2.187080

30 C 7.812362 8.173031 7.542408 8.595946 9.857586

31 H 8.341135 8.221194 7.180120 7.837551 9.295980

32 C 8.726224 7.835661 6.468969 6.115259 7.486765

33 H 7.496672 6.322993 5.083397 4.177116 5.222621

34 H 4.140375 5.461234 6.368004 7.611688 7.653067

35 H 3.084177 4.339554 5.412523 6.530397 6.378476

36 H 3.084177 4.339554 5.412523 6.530397 6.378476

37 H 5.567276 4.327079 4.127840 2.932655 2.135341

38 H 5.567276 4.327079 4.127840 2.932655 2.135341

39 H 5.231571 4.163424 4.455865 3.537142 2.140587

40 H 7.789108 8.250058 7.724622 8.836188 10.033941

41 H 7.789108 8.250058 7.724622 8.836188 10.033941

42 H 8.824242 9.111793 8.392016 9.366917 10.687814

43 H 9.073045 8.253658 6.897896 6.648318 8.045013

44 H 9.073045 8.253658 6.897896 6.648318 8.045013

45 H 9.360885 8.370549 7.018653 6.468771 7.731387

11 12 13 14 15

11 C 0.000000

12 N 6.835422 0.000000

13 C 8.426066 2.483089 0.000000

14 C 8.518429 3.539757 1.349463 0.000000

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16 N 6.243192 2.416962 2.320876 2.304642 1.366977

17 C 7.002440 1.316548 1.503275 2.285716 2.232688

18 N 7.286949 4.761318 3.553975 2.478932 1.321415

19 N 4.987581 5.009364 5.003578 4.414063 2.932276

20 C 6.342511 5.332524 4.659534 3.752875 2.374724

21 C 6.904913 6.799191 6.018822 4.978997 3.730013

22 C 6.000117 7.260324 6.907682 6.022484 4.638533

23 C 4.654393 6.269215 6.368170 5.729227 4.253341

24 N 3.539757 6.778060 7.303638 6.835422 5.356173

25 Zn 4.259215 3.389030 4.274214 4.259215 3.007093

26 C 5.347825 5.015705 7.486765 8.386362 7.835661

27 H 7.066127 2.864714 5.222621 6.386513 6.322993

28 C 2.571865 8.747791 9.857586 9.618103 8.173031

29 H 1.081221 7.535825 9.295980 9.474889 8.221194

30 C 9.618103 3.047585 1.485391 2.571865 3.758638

31 H 9.474889 4.565428 2.187080 1.081221 2.271108

32 C 8.386362 7.775746 6.567697 5.347825 4.397284

33 H 6.386513 8.318674 7.981098 7.066127 5.704459

34 H 6.439073 5.254738 7.731387 8.753635 8.370549

35 H 5.120889 5.614980 8.045013 8.884126 8.253658

36 H 5.120889 5.614980 8.045013 8.884126 8.253658

37 H 3.276105 9.077042 10.033941 9.708285 8.250058

38 H 3.276105 9.077042 10.033941 9.708285 8.250058

39 H 2.755345 9.398505 10.687814 10.533924 9.111793

40 H 9.708285 3.046345 2.135341 3.276105 4.327079

41 H 9.708285 3.046345 2.135341 3.276105 4.327079

42 H 10.533924 4.112519 2.140587 2.755345 4.163424

43 H 8.884126 7.766107 6.378476 5.120889 4.339554

44 H 8.884126 7.766107 6.378476 5.120889 4.339554

45 H 8.753635 8.784346 7.653067 6.439073 5.461234

16 17 18 19 20

16 N 0.000000

17 C 1.364147 0.000000

18 N 2.414707 3.517470 0.000000

19 N 2.835202 4.185474 2.439601 0.000000

20 C 2.928268 4.250567 1.365162 1.356050 0.000000

21 C 4.395732 5.710924 2.501713 2.293931 1.467676

22 C 4.972464 6.335776 3.583255 2.281679 2.272301

23 C 4.188704 5.526267 3.547452 1.366172 2.219721

24 N 5.013616 6.262155 4.823258 2.440372 3.544706

25 Zn 2.000875 2.998069 3.388430 2.009739 3.002474

26 C 6.468969 6.115259 8.726224 7.542457 8.592477

27 H 5.083397 4.177116 7.496672 7.177448 7.833941

28 C 7.542408 8.595946 7.812362 5.378279 6.577440

29 H 7.180120 7.837551 8.341135 6.063934 7.419574

30 C 3.736262 2.631944 4.976996 6.480184 6.132499

31 H 3.333711 3.348191 2.837099 5.095836 4.200044

32 C 5.367302 6.574870 3.076428 3.719935 2.616776

33 H 6.049956 7.413800 4.604206 3.316358 3.330909

34 H 7.018653 6.468771 9.360885 8.383087 9.353943

35 H 6.897896 6.648318 9.073045 7.740553 8.847582

36 H 6.897896 6.648318 9.073045 7.740553 8.847582

37 H 7.724622 8.836188 7.789108 5.406122 6.516122

38 H 7.724622 8.836188 7.789108 5.406122 6.516122

39 H 8.392016 9.366917 8.824242 6.384716 7.618590

40 H 4.127840 2.932655 5.567276 6.895926 6.653698

41 H 4.127840 2.932655 5.567276 6.895926 6.653698

42 H 4.455865 3.537142 5.231571 7.041815 6.500803

43 H 5.412523 6.530397 3.084177 4.126902 2.935876

44 H 5.412523 6.530397 3.084177 4.126902 2.935876

45 H 6.368004 7.611688 4.140375 4.428083 3.512749

21 22 23 24 25

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22 C 1.374729 0.000000

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27 H 9.260515 9.447590 8.221348 8.318674 5.217082

28 C 6.579040 5.335776 4.414390 3.047585 5.605380

29 H 7.980449 7.047753 5.722778 4.565428 5.227846

30 C 7.466138 8.388086 7.845976 8.747791 5.605380

31 H 5.211486 6.401549 6.333732 7.535825 5.227846

32 C 1.488723 2.588862 3.740979 5.015705 5.596806

33 H 2.205708 1.081129 2.247425 2.864714 5.217082

34 H 10.649086 10.497115 9.108070 8.784346 6.395544

35 H 10.023061 9.694207 8.270294 7.766107 5.868108

36 H 10.023061 9.694207 8.270294 7.766107 5.868108

37 H 6.377324 5.096275 4.339103 3.046345 5.860966

38 H 6.377324 5.096275 4.339103 3.046345 5.860966

39 H 7.664965 6.426709 5.481311 4.112519 6.413800

40 H 8.013613 8.872415 8.251038 9.077042 5.860966

41 H 8.013613 8.872415 8.251038 9.077042 5.860966

42 H 7.727120 8.772741 8.392526 9.398505 6.413800

43 H 2.143371 3.298734 4.321716 5.614980 5.868108

44 H 2.143371 3.298734 4.321716 5.614980 5.868108

45 H 2.142270 2.757979 4.129723 5.254738 6.395544

26 27 28 29 30

26 C 0.000000

27 H 2.990269 0.000000

28 C 7.918559 9.459229 0.000000

29 H 5.275060 7.390081 2.985758 0.000000

30 C 7.923729 5.272518 11.210760 10.420488 0.000000

31 H 9.459544 7.381282 10.420488 10.455692 2.985758

32 C 11.193612 10.399166 7.923729 9.459544 7.918559

33 H 10.399166 10.434164 5.272518 7.381282 9.459229

34 H 1.091360 2.740399 9.009557 6.350522 7.967084

35 H 1.095140 3.745163 7.662532 4.936512 8.543744

36 H 1.095140 3.745163 7.662532 4.936512 8.543744

37 H 8.530128 9.945101 1.094733 3.738520 11.416829

38 H 8.530128 9.945101 1.094733 3.738520 11.416829

39 H 7.978710 9.820574 1.090942 2.750613 11.996836

40 H 7.654230 4.922673 11.416829 10.458779 1.094733

41 H 7.654230 4.922673 11.416829 10.458779 1.094733

42 H 9.014562 6.345540 11.996836 11.374029 1.090942

43 H 11.415714 10.453661 8.543744 9.957960 7.662532

44 H 11.415714 10.453661 8.543744 9.957960 7.662532

45 H 11.969268 11.346015 7.967084 9.804977 9.009557

31 32 33 34 35

31 H 0.000000

32 C 5.275060 0.000000

33 H 7.390081 2.990269 0.000000

34 H 9.804977 11.969268 11.346015 0.000000

35 H 9.957960 11.415714 10.453661 1.771815 0.000000

36 H 9.957960 11.415714 10.453661 1.771815 1.754159

37 H 10.458779 7.654230 4.922673 9.614153 8.201042

38 H 10.458779 7.654230 4.922673 9.614153 8.386494

39 H 11.374029 9.014562 6.345540 9.064304 7.644665

40 H 3.738520 8.530128 9.945101 7.620753 8.199875

41 H 3.738520 8.530128 9.945101 7.620753 8.385353

42 H 2.750613 7.978710 9.820574 9.050857 9.628195

43 H 4.936512 1.095140 3.745163 12.146440 11.604382

44 H 4.936512 1.095140 3.745163 12.146440 11.736216

45 H 6.350522 1.091360 2.740399 12.791087 12.146440

36 37 38 39 40

36 H 0.000000

37 H 8.386494 0.000000

38 H 8.201042 1.753664 0.000000

39 H 7.644665 1.774808 1.774808 0.000000

40 H 8.385353 11.590011 11.721932 12.158354 0.000000

41 H 8.199875 11.721932 11.590011 12.158354 1.753664

42 H 9.628195 12.158354 12.158354 12.827600 1.774808

43 H 11.736216 8.199875 8.385353 9.628195 8.201042

44 H 11.604382 8.385353 8.199875 9.628195 8.386494

45 H 12.146440 7.620753 7.620753 9.050857 9.614153

41 42 43 44 45

41 H 0.000000

42 H 1.774808 0.000000

43 H 8.386494 7.644665 0.000000

44 H 8.201042 7.644665 1.754159 0.000000

45 H 9.614153 9.064304 1.771815 1.771815 0.000000

Stoichiometry C20H16N8Zn(3)

Framework group C2H[O(Zn),SGH(C20H8N8),X(H8)]

Deg. of freedom 41

Full point group C2H NOp 4

RotChk: IX=0 Diff= 3.24D-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 2.805774 -1.109249 0.000000

2 7 0 2.009739 0.001045 0.000000

3 6 0 2.789593 1.110414 0.000000

4 6 0 4.196737 0.693257 0.000000

5 6 0 4.186956 -0.681437 0.000000

6 7 0 2.379367 2.412482 0.000000

7 6 0 1.113969 2.793148 0.000000

8 7 0 0.000000 2.000875 0.000000

9 6 0 -1.118688 2.781538 0.000000

10 6 0 -0.680850 4.219639 0.000000

11 6 0 0.668548 4.206418 0.000000

12 7 0 2.381951 -2.410775 0.000000

13 6 0 0.680850 -4.219639 0.000000

14 6 0 -0.668548 -4.206418 0.000000

15 6 0 -1.113969 -2.793148 0.000000

16 7 0 -0.000000 -2.000875 0.000000

17 6 0 1.118688 -2.781538 0.000000

18 7 0 -2.379367 -2.412482 0.000000

19 7 0 -2.009739 -0.001045 0.000000

20 6 0 -2.789593 -1.110414 0.000000

21 6 0 -4.196737 -0.693257 0.000000

22 6 0 -4.186956 0.681437 0.000000

23 6 0 -2.805774 1.109249 0.000000

24 7 0 -2.381951 2.410775 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 5.354420 1.629241 0.000000

27 1 0 5.040848 -1.344542 0.000000

28 6 0 -1.628236 5.363686 0.000000

29 1 0 1.341297 5.052850 0.000000

30 6 0 1.628236 -5.363686 0.000000

31 1 0 -1.341297 -5.052850 0.000000

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35 1 0 5.333440 2.284696 0.877080

36 1 0 5.333440 2.284696 -0.877080

37 1 0 -2.282625 5.326511 0.876832

38 1 0 -2.282625 5.326511 -0.876832

39 1 0 -1.100763 6.318635 0.000000

40 1 0 2.282625 -5.326511 0.876832

41 1 0 2.282625 -5.326511 -0.876832

42 1 0 1.100763 -6.318635 0.000000

43 1 0 -5.333440 -2.284696 0.877080

44 1 0 -5.333440 -2.284696 -0.877080

45 1 0 -6.302272 -1.088275 0.000000

---------------------------------------------------------------------

Rotational constants (GHZ): 0.1829582 0.1818963 0.0914175

Leave Link 202 at Tue Sep 17 14:42:37 2019, MaxMem= 2415919104 cpu: 0.2

(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:

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The electronic state is 3-BU.

Alpha occ. eigenvalues -- -14.31421 -14.31421 -14.31299 -14.31299 -14.30673

Alpha occ. eigenvalues -- -14.30673 -14.30228 -14.30227 -10.26067 -10.26067

Alpha occ. eigenvalues -- -10.25917 -10.25917 -10.25088 -10.25088 -10.25000

Alpha occ. eigenvalues -- -10.25000 -10.19696 -10.19696 -10.18741 -10.18741

Alpha occ. eigenvalues -- -10.17876 -10.17875 -10.16864 -10.16864 -10.16527

Alpha occ. eigenvalues -- -10.16527 -10.16238 -10.16237 -1.00619 -0.99284

Alpha occ. eigenvalues -- -0.99131 -0.96506 -0.94218 -0.90418 -0.89718

Alpha occ. eigenvalues -- -0.86739 -0.80280 -0.79980 -0.79265 -0.79245

Alpha occ. eigenvalues -- -0.75473 -0.72393 -0.71895 -0.70622 -0.69238

Alpha occ. eigenvalues -- -0.68309 -0.67926 -0.63262 -0.61200 -0.59071

Alpha occ. eigenvalues -- -0.57910 -0.57540 -0.57051 -0.56895 -0.55798

Alpha occ. eigenvalues -- -0.55744 -0.54759 -0.54311 -0.54243 -0.53733

Alpha occ. eigenvalues -- -0.51988 -0.50754 -0.50604 -0.49216 -0.48739

Alpha occ. eigenvalues -- -0.46731 -0.45212 -0.45119 -0.44536 -0.43873

Alpha occ. eigenvalues -- -0.43254 -0.43240 -0.42869 -0.40916 -0.40839

Alpha occ. eigenvalues -- -0.40566 -0.40200 -0.39757 -0.39565 -0.39512

Alpha occ. eigenvalues -- -0.39366 -0.38079 -0.38064 -0.37951 -0.37457

Alpha occ. eigenvalues -- -0.37192 -0.36694 -0.33056 -0.33018 -0.32721

Alpha occ. eigenvalues -- -0.32310 -0.30898 -0.28096 -0.28043 -0.26783

Alpha occ. eigenvalues -- -0.26338 -0.25879 -0.25689 -0.25448 -0.25032

Alpha occ. eigenvalues -- -0.25009 -0.22638 -0.15796

Alpha virt. eigenvalues -- -0.10623 -0.05742 0.01730 0.03301 0.03820

Alpha virt. eigenvalues -- 0.03899 0.04504 0.04530 0.05251 0.05519

Alpha virt. eigenvalues -- 0.06969 0.07027 0.08204 0.08241 0.08839

Alpha virt. eigenvalues -- 0.09291 0.09710 0.09985 0.10083 0.10211

Alpha virt. eigenvalues -- 0.10398 0.10469 0.12868 0.13493 0.13560

Alpha virt. eigenvalues -- 0.13656 0.13686 0.13707 0.13782 0.14174

Alpha virt. eigenvalues -- 0.17893 0.19835 0.20338 0.20468 0.20718

Alpha virt. eigenvalues -- 0.20906 0.21409 0.21803 0.21999 0.22148

Alpha virt. eigenvalues -- 0.22611 0.22874 0.23344 0.25632 0.27149

Alpha virt. eigenvalues -- 0.27455 0.27995 0.28444 0.28827 0.28977

Alpha virt. eigenvalues -- 0.29998 0.30012 0.31239 0.31317 0.31612

Alpha virt. eigenvalues -- 0.31760 0.31876 0.31922 0.32017 0.32638

Alpha virt. eigenvalues -- 0.34771 0.35110 0.35382 0.35937 0.37391

Alpha virt. eigenvalues -- 0.37740 0.37797 0.38696 0.38702 0.38837

Alpha virt. eigenvalues -- 0.39981 0.40030 0.40456 0.40910 0.41508

Alpha virt. eigenvalues -- 0.43193 0.43398 0.43781 0.43912 0.43950

Alpha virt. eigenvalues -- 0.45536 0.46040 0.46321 0.47026 0.48030

Alpha virt. eigenvalues -- 0.48609 0.48842 0.49277 0.49376 0.49486

Alpha virt. eigenvalues -- 0.49801 0.51419 0.51471 0.51482 0.51732

Alpha virt. eigenvalues -- 0.52865 0.53730 0.53939 0.54008 0.54641

Alpha virt. eigenvalues -- 0.56019 0.56453 0.56878 0.56879 0.57279

Alpha virt. eigenvalues -- 0.57539 0.57570 0.58292 0.58451 0.58456

Alpha virt. eigenvalues -- 0.58941 0.59498 0.59680 0.59974 0.60507

Alpha virt. eigenvalues -- 0.61607 0.62635 0.62870 0.63246 0.63291

Alpha virt. eigenvalues -- 0.63577 0.63610 0.65128 0.65256 0.65373

Alpha virt. eigenvalues -- 0.68009 0.68195 0.68794 0.68869 0.69104

Alpha virt. eigenvalues -- 0.69350 0.69531 0.69982 0.71080 0.71594

Alpha virt. eigenvalues -- 0.73102 0.73441 0.74038 0.74666 0.75337

Alpha virt. eigenvalues -- 0.75921 0.76205 0.77536 0.78263 0.79032

Alpha virt. eigenvalues -- 0.79715 0.80037 0.80703 0.81030 0.81034

Alpha virt. eigenvalues -- 0.81067 0.81979 0.82404 0.82567 0.84993

Alpha virt. eigenvalues -- 0.85258 0.85535 0.86948 0.88715 0.88807

Alpha virt. eigenvalues -- 0.88874 0.89739 0.94379 0.96282 0.97290

Alpha virt. eigenvalues -- 0.97513 0.98122 0.99961 1.00250 1.00755

Alpha virt. eigenvalues -- 1.03228 1.03423 1.04431 1.04878 1.05362

Alpha virt. eigenvalues -- 1.06682 1.08277 1.08310 1.08675 1.10443

Alpha virt. eigenvalues -- 1.10666 1.13248 1.13623 1.13752 1.13828

Alpha virt. eigenvalues -- 1.13872 1.13964 1.14095 1.14510 1.14958

Alpha virt. eigenvalues -- 1.18271 1.18715 1.19050 1.19184 1.20579

Alpha virt. eigenvalues -- 1.20702 1.21387 1.23427 1.24099 1.27685

Alpha virt. eigenvalues -- 1.28541 1.29014 1.29286 1.31167 1.35999

Alpha virt. eigenvalues -- 1.36186 1.37061 1.38086 1.39148 1.40522

Alpha virt. eigenvalues -- 1.40877 1.41202 1.41940 1.42227 1.43714

Alpha virt. eigenvalues -- 1.45006 1.49477 1.49590 1.49958 1.50890

Alpha virt. eigenvalues -- 1.50969 1.51200 1.51312 1.51960 1.52017

Alpha virt. eigenvalues -- 1.52131 1.52751 1.53932 1.54726 1.55196

Alpha virt. eigenvalues -- 1.55506 1.56069 1.56202 1.57132 1.58562

Alpha virt. eigenvalues -- 1.60270 1.60314 1.61209 1.61674 1.62794

Alpha virt. eigenvalues -- 1.62954 1.63269 1.67065 1.67900 1.68255

Alpha virt. eigenvalues -- 1.68378 1.68925 1.69230 1.69618 1.70477

Alpha virt. eigenvalues -- 1.70980 1.72875 1.73912 1.75376 1.75964

Alpha virt. eigenvalues -- 1.76205 1.79436 1.79731 1.79900 1.80589

Alpha virt. eigenvalues -- 1.84950 1.86406 1.86763 1.86946 1.88558

Alpha virt. eigenvalues -- 1.89714 1.90679 1.90705 1.91617 1.93731

Alpha virt. eigenvalues -- 1.95317 1.95915 1.96730 1.96969 2.00737

Alpha virt. eigenvalues -- 2.00777 2.01130 2.01444 2.01969 2.02071

Alpha virt. eigenvalues -- 2.02072 2.03023 2.05181 2.06928 2.07964

Alpha virt. eigenvalues -- 2.08397 2.09841 2.12141 2.12873 2.14833

Alpha virt. eigenvalues -- 2.15480 2.15815 2.17326 2.17953 2.19948

Alpha virt. eigenvalues -- 2.27538 2.27924 2.29424 2.29458 2.30106

Alpha virt. eigenvalues -- 2.30486 2.32804 2.33758 2.34938 2.34987

Alpha virt. eigenvalues -- 2.35428 2.36246 2.36931 2.37820 2.38313

Alpha virt. eigenvalues -- 2.38756 2.39455 2.39764 2.39878 2.43840

Alpha virt. eigenvalues -- 2.47413 2.47756 2.48009 2.48048 2.48089

Alpha virt. eigenvalues -- 2.48513 2.48836 2.49282 2.55047 2.55417

Alpha virt. eigenvalues -- 2.56209 2.56586 2.57734 2.58680 2.59104

Alpha virt. eigenvalues -- 2.59892 2.60405 2.62995 2.63576 2.64811

Alpha virt. eigenvalues -- 2.66409 2.67545 2.70241 2.70580 2.71440

Alpha virt. eigenvalues -- 2.71878 2.72298 2.72900 2.74923 2.75743

Alpha virt. eigenvalues -- 2.76237 2.79119 2.82531 2.83277 2.83566

Alpha virt. eigenvalues -- 2.83575 2.83872 2.84501 2.84710 2.84949

Alpha virt. eigenvalues -- 2.91394 2.91745 2.92697 2.93472 2.95885

Alpha virt. eigenvalues -- 2.96236 2.97216 3.01096 3.02614 3.03377

Alpha virt. eigenvalues -- 3.05025 3.06071 3.11376 3.12571 3.13066

Alpha virt. eigenvalues -- 3.13160 3.13677 3.13725 3.14031 3.15078

Alpha virt. eigenvalues -- 3.15843 3.15896 3.17826 3.18255 3.19830

Alpha virt. eigenvalues -- 3.20389 3.21101 3.22479 3.24460 3.26719

Alpha virt. eigenvalues -- 3.27895 3.28212 3.28245 3.29880 3.30976

Alpha virt. eigenvalues -- 3.36216 3.38044 3.38786 3.39194 3.39356

Alpha virt. eigenvalues -- 3.52857 3.56558 3.57595 3.69582 3.72054

Alpha virt. eigenvalues -- 3.72173 3.72501 3.75870 3.77707 3.77820

Alpha virt. eigenvalues -- 3.78800 3.79038 3.81302 3.81925 3.82106

Alpha virt. eigenvalues -- 3.87117 3.87554 3.87888 3.88268 3.91146

Alpha virt. eigenvalues -- 4.04325 4.04950 4.05044 4.05919 4.11201

Alpha virt. eigenvalues -- 4.12058 4.12333 4.18430 4.28520 4.35997

Alpha virt. eigenvalues -- 4.36284 4.38272 4.46600 4.51190 4.61010

Alpha virt. eigenvalues -- 4.61378 4.99400 5.02425 5.03138 5.11739

Alpha virt. eigenvalues -- 5.14290 5.31558 5.32442 5.48495 7.78289

Alpha virt. eigenvalues -- 7.78444 7.89566 7.95293 8.23001 11.19761

Alpha virt. eigenvalues -- 23.42635 23.44468 23.45915 23.46692 23.67023

Alpha virt. eigenvalues -- 23.67545 23.67592 23.67630 23.80527 23.80797

Alpha virt. eigenvalues -- 23.82863 23.83335 23.84994 23.85731 23.87263

Alpha virt. eigenvalues -- 23.87479 24.09477 24.09527 24.15784 24.15940

Alpha virt. eigenvalues -- 35.56776 35.60732 35.61478 35.61936 35.67898

Alpha virt. eigenvalues -- 35.68818 35.68877 35.68973

Beta occ. eigenvalues -- -14.31399 -14.31399 -14.31249 -14.31249 -14.30829

Beta occ. eigenvalues -- -14.30829 -14.30131 -14.30131 -10.25863 -10.25863

Beta occ. eigenvalues -- -10.25699 -10.25699 -10.24619 -10.24619 -10.24555

Beta occ. eigenvalues -- -10.24555 -10.19652 -10.19652 -10.18544 -10.18544

Beta occ. eigenvalues -- -10.17881 -10.17881 -10.16838 -10.16838 -10.16528

Beta occ. eigenvalues -- -10.16528 -10.16247 -10.16247 -1.00173 -0.98873

Beta occ. eigenvalues -- -0.98644 -0.96099 -0.93755 -0.90099 -0.89331

Beta occ. eigenvalues -- -0.86555 -0.80103 -0.79839 -0.78998 -0.78993

Beta occ. eigenvalues -- -0.74702 -0.71819 -0.71681 -0.70504 -0.68988

Beta occ. eigenvalues -- -0.67823 -0.67589 -0.62813 -0.60726 -0.58970

Beta occ. eigenvalues -- -0.57766 -0.57467 -0.56780 -0.56621 -0.55761

Beta occ. eigenvalues -- -0.55740 -0.54582 -0.54219 -0.53917 -0.53425

Beta occ. eigenvalues -- -0.51782 -0.50608 -0.50391 -0.48976 -0.48603

Beta occ. eigenvalues -- -0.45474 -0.44471 -0.44261 -0.43819 -0.43634

Beta occ. eigenvalues -- -0.43146 -0.42777 -0.42473 -0.40610 -0.40431

Beta occ. eigenvalues -- -0.40048 -0.40033 -0.39688 -0.39395 -0.39198

Beta occ. eigenvalues -- -0.38321 -0.37908 -0.37772 -0.37362 -0.37090

Beta occ. eigenvalues -- -0.36720 -0.36515 -0.32868 -0.32673 -0.31578

Beta occ. eigenvalues -- -0.30734 -0.30406 -0.27976 -0.27925 -0.26304

Beta occ. eigenvalues -- -0.26246 -0.25629 -0.25371 -0.25079 -0.24611

Beta occ. eigenvalues -- -0.24468

Beta virt. eigenvalues -- -0.16276 -0.09848 -0.09345 -0.03888 0.03400

Beta virt. eigenvalues -- 0.03858 0.04560 0.04636 0.05032 0.05509

Beta virt. eigenvalues -- 0.05556 0.06459 0.06982 0.07053 0.08238

Beta virt. eigenvalues -- 0.08299 0.09323 0.10006 0.10121 0.10280

Beta virt. eigenvalues -- 0.10295 0.10670 0.11740 0.11914 0.12879

Beta virt. eigenvalues -- 0.13582 0.13682 0.13683 0.13706 0.13991

Beta virt. eigenvalues -- 0.14321 0.14540 0.18351 0.20065 0.20636

Beta virt. eigenvalues -- 0.20698 0.20930 0.21244 0.21827 0.22146

Beta virt. eigenvalues -- 0.22169 0.22426 0.23103 0.23180 0.23879

Beta virt. eigenvalues -- 0.25989 0.27506 0.27674 0.28136 0.28669

Beta virt. eigenvalues -- 0.29333 0.29421 0.30343 0.30419 0.31334

Beta virt. eigenvalues -- 0.31383 0.31817 0.32026 0.32044 0.32166

Beta virt. eigenvalues -- 0.32231 0.32834 0.34876 0.35420 0.35698

Beta virt. eigenvalues -- 0.36195 0.37645 0.38030 0.38044 0.39152

Beta virt. eigenvalues -- 0.39442 0.39948 0.40179 0.40227 0.40790

Beta virt. eigenvalues -- 0.41207 0.42160 0.43421 0.44060 0.44205

Beta virt. eigenvalues -- 0.44241 0.44813 0.45810 0.46531 0.46682

Beta virt. eigenvalues -- 0.47290 0.48267 0.48855 0.49334 0.49514

Beta virt. eigenvalues -- 0.49649 0.49692 0.50095 0.51709 0.51954

Beta virt. eigenvalues -- 0.52143 0.52310 0.53540 0.53948 0.54085

Beta virt. eigenvalues -- 0.54122 0.54741 0.56163 0.56631 0.57019

Beta virt. eigenvalues -- 0.57027 0.57389 0.57699 0.58025 0.58474

Beta virt. eigenvalues -- 0.58556 0.58610 0.59084 0.59560 0.59872

Beta virt. eigenvalues -- 0.60142 0.60670 0.61786 0.62796 0.63107

Beta virt. eigenvalues -- 0.63731 0.63794 0.63905 0.63925 0.65305

Beta virt. eigenvalues -- 0.65390 0.65478 0.68397 0.68707 0.68919

Beta virt. eigenvalues -- 0.69015 0.69376 0.69478 0.69721 0.70229

Beta virt. eigenvalues -- 0.71353 0.71951 0.73415 0.73716 0.74272

Beta virt. eigenvalues -- 0.74840 0.75617 0.76118 0.76367 0.77761

Beta virt. eigenvalues -- 0.78497 0.79106 0.79907 0.80376 0.81106

Beta virt. eigenvalues -- 0.81230 0.81277 0.81341 0.82183 0.82552

Beta virt. eigenvalues -- 0.82709 0.85148 0.85411 0.85729 0.87074

Beta virt. eigenvalues -- 0.88869 0.88929 0.89206 0.89934 0.94635

Beta virt. eigenvalues -- 0.96400 0.97388 0.97774 0.98303 1.00096

Beta virt. eigenvalues -- 1.00520 1.01386 1.03788 1.03903 1.04552

Beta virt. eigenvalues -- 1.05162 1.05600 1.07011 1.08482 1.08710

Beta virt. eigenvalues -- 1.09585 1.10749 1.10993 1.13364 1.13929

Beta virt. eigenvalues -- 1.13993 1.14303 1.14318 1.14718 1.14935

Beta virt. eigenvalues -- 1.15166 1.16041 1.18584 1.19148 1.19285

Beta virt. eigenvalues -- 1.19697 1.20859 1.21438 1.22163 1.23517

Beta virt. eigenvalues -- 1.24212 1.27851 1.29255 1.29284 1.29484

Beta virt. eigenvalues -- 1.31358 1.36775 1.37003 1.37404 1.39036

Beta virt. eigenvalues -- 1.39347 1.41039 1.41250 1.41382 1.42278

Beta virt. eigenvalues -- 1.42571 1.44009 1.45323 1.49579 1.49665

Beta virt. eigenvalues -- 1.50062 1.50951 1.51040 1.51324 1.51412

Beta virt. eigenvalues -- 1.52030 1.52105 1.52175 1.52897 1.54522

Beta virt. eigenvalues -- 1.54922 1.55381 1.55666 1.56252 1.56580

Beta virt. eigenvalues -- 1.57463 1.59011 1.60458 1.60578 1.61797

Beta virt. eigenvalues -- 1.61806 1.62976 1.63252 1.63603 1.67220

Beta virt. eigenvalues -- 1.68476 1.68512 1.68607 1.69108 1.69439

Beta virt. eigenvalues -- 1.69857 1.71018 1.71176 1.73889 1.74154

Beta virt. eigenvalues -- 1.75656 1.76467 1.76968 1.79748 1.79977

Beta virt. eigenvalues -- 1.80367 1.80985 1.85162 1.86680 1.87022

Beta virt. eigenvalues -- 1.87447 1.88813 1.90143 1.90895 1.91550

Beta virt. eigenvalues -- 1.92297 1.94140 1.95787 1.96282 1.97120

Beta virt. eigenvalues -- 1.97613 2.01355 2.01400 2.02177 2.02183

Beta virt. eigenvalues -- 2.02244 2.02246 2.02281 2.03486 2.05404

Beta virt. eigenvalues -- 2.07378 2.08365 2.08605 2.10012 2.12585

Beta virt. eigenvalues -- 2.13333 2.15220 2.16055 2.16289 2.17952

Beta virt. eigenvalues -- 2.18122 2.20507 2.27673 2.28640 2.29479

Beta virt. eigenvalues -- 2.29570 2.30178 2.30833 2.33405 2.34128

Beta virt. eigenvalues -- 2.35012 2.35065 2.35549 2.36322 2.37540

Beta virt. eigenvalues -- 2.37933 2.38840 2.38959 2.39900 2.39911

Beta virt. eigenvalues -- 2.40466 2.44008 2.47657 2.48002 2.48284

Beta virt. eigenvalues -- 2.48298 2.48385 2.48677 2.49318 2.49544

Beta virt. eigenvalues -- 2.54964 2.55485 2.56538 2.56743 2.57874

Beta virt. eigenvalues -- 2.58839 2.59764 2.60335 2.61357 2.63635

Beta virt. eigenvalues -- 2.63649 2.65019 2.67107 2.67640 2.70868

Beta virt. eigenvalues -- 2.71148 2.72001 2.72008 2.72453 2.73069

Beta virt. eigenvalues -- 2.76071 2.76832 2.77337 2.80276 2.83454

Beta virt. eigenvalues -- 2.83671 2.84269 2.84644 2.84724 2.84857

Beta virt. eigenvalues -- 2.85074 2.85194 2.91532 2.91899 2.92857

Beta virt. eigenvalues -- 2.94166 2.96004 2.96798 2.98514 3.02230

Beta virt. eigenvalues -- 3.02752 3.03479 3.05199 3.06240 3.11485

Beta virt. eigenvalues -- 3.12690 3.13217 3.13268 3.13763 3.13921

Beta virt. eigenvalues -- 3.14185 3.15251 3.15921 3.16078 3.17956

Beta virt. eigenvalues -- 3.18331 3.19970 3.20511 3.21256 3.22593

Beta virt. eigenvalues -- 3.24573 3.26814 3.27994 3.28366 3.28379

Beta virt. eigenvalues -- 3.29989 3.31180 3.36374 3.38125 3.38826

Beta virt. eigenvalues -- 3.39336 3.39466 3.53111 3.56752 3.57855

Beta virt. eigenvalues -- 3.69787 3.72303 3.72425 3.72707 3.76073

Beta virt. eigenvalues -- 3.78008 3.78026 3.78989 3.79313 3.81571

Beta virt. eigenvalues -- 3.81800 3.82560 3.87202 3.87974 3.88212

Beta virt. eigenvalues -- 3.88343 3.91264 4.04454 4.05073 4.05364

Beta virt. eigenvalues -- 4.06237 4.11326 4.12173 4.12557 4.18664

Beta virt. eigenvalues -- 4.28690 4.36300 4.36625 4.38671 4.46795

Beta virt. eigenvalues -- 4.51291 4.61193 4.61436 4.99739 5.02695

Beta virt. eigenvalues -- 5.03558 5.12076 5.14652 5.31905 5.32814

Beta virt. eigenvalues -- 5.48855 7.78274 7.78482 7.89565 7.95296

Beta virt. eigenvalues -- 8.23005 11.19768 23.42708 23.44496 23.46053

Beta virt. eigenvalues -- 23.46789 23.67076 23.67600 23.67622 23.67663

Beta virt. eigenvalues -- 23.80779 23.81066 23.83292 23.83768 23.85466

Beta virt. eigenvalues -- 23.86223 23.87554 23.87741 24.09612 24.09661

Beta virt. eigenvalues -- 24.15810 24.15967 35.56786 35.60815 35.61354

Beta virt. eigenvalues -- 35.61886 35.67940 35.68841 35.68922 35.68998

Condensed to atoms (all electrons):

1 2 3 4 5 6

1 C 4.656557 0.401444 -0.137108 -0.056288 0.443544 -0.001110

2 N 0.401444 7.103763 0.388418 -0.066013 -0.097230 -0.076898

3 C -0.137108 0.388418 4.679180 0.427061 -0.072537 0.513358

4 C -0.056288 -0.066013 0.427061 5.066337 0.600926 -0.078321

5 C 0.443544 -0.097230 -0.072537 0.600926 5.137975 0.005152

6 N -0.001110 -0.076898 0.513358 -0.078321 0.005152 6.615756

7 C -0.000893 -0.002802 -0.095379 0.003234 -0.000411 0.557075

8 N 0.000416 -0.020555 -0.004265 -0.000051 -0.000208 -0.080548

9 C -0.000002 0.000426 -0.001071 0.000016 -0.000003 0.000579

10 C -0.000003 -0.000082 0.000073 0.000016 0.000000 0.002921

11 C 0.000018 0.000166 0.004800 -0.000279 0.000011 -0.043009

12 N 0.467184 -0.069642 0.000871 0.004231 -0.045532 -0.000140

13 C 0.005460 -0.000186 0.000019 0.000015 -0.000340 -0.000000

14 C -0.000270 -0.000193 -0.000003 0.000000 0.000010 -0.000000

15 C -0.001292 0.000539 -0.000003 -0.000003 0.000019 -0.000001

16 N -0.003425 -0.020616 0.000238 -0.000100 0.000375 -0.000003

17 C -0.097469 -0.003533 -0.000705 0.000082 0.003504 -0.000023

18 N -0.000025 -0.000005 -0.000001 -0.000000 -0.000000 0.000000

19 N 0.000154 -0.003150 0.000214 0.000002 0.000003 -0.000005

20 C -0.000046 0.000214 -0.000014 -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 -0.000006 0.000154 -0.000046 -0.000000 -0.000000 -0.000025

24 N -0.000001 -0.000005 -0.000031 -0.000000 -0.000000 -0.000152

25 Zn -0.016268 0.117257 -0.017474 -0.000715 -0.000536 -0.005424

26 C 0.009545 0.009105 -0.071206 0.267360 -0.055781 0.014466

27 H -0.050019 0.006416 0.009685 -0.043748 0.397359 -0.000016

28 C 0.000000 0.000000 0.000003 -0.000000 0.000000 -0.000019

29 H 0.000001 0.000075 -0.000226 -0.000155 -0.000004 0.006832

30 C -0.000615 0.000062 0.000000 -0.000000 -0.000035 0.000000

31 H 0.000014 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 0.000220 -0.000238 0.006230 -0.041580 -0.005423 0.000090

35 H -0.000085 0.000424 -0.005778 -0.045436 -0.000040 0.004378

36 H -0.000085 0.000424 -0.005778 -0.045436 -0.000040 0.004378

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 -0.000108 0.000015 -0.000000 0.000000 -0.000023 0.000000

41 H -0.000108 0.000015 -0.000000 0.000000 -0.000023 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 -0.000893 0.000416 -0.000002 -0.000003 0.000018 0.467184

2 N -0.002802 -0.020555 0.000426 -0.000082 0.000166 -0.069642

3 C -0.095379 -0.004265 -0.001071 0.000073 0.004800 0.000871

4 C 0.003234 -0.000051 0.000016 0.000016 -0.000279 0.004231

5 C -0.000411 -0.000208 -0.000003 0.000000 0.000011 -0.045532

6 N 0.557075 -0.080548 0.000579 0.002921 -0.043009 -0.000140

7 C 4.572749 0.397472 -0.123055 -0.051652 0.388237 -0.000016

8 N 0.397472 7.174850 0.375430 -0.061284 -0.096878 -0.000003

9 C -0.123055 0.375430 4.607820 0.367689 -0.065520 -0.000001

10 C -0.051652 -0.061284 0.367689 5.058232 0.641035 -0.000000

11 C 0.388237 -0.096878 -0.065520 0.641035 5.120709 -0.000000

12 N -0.000016 -0.000003 -0.000001 -0.000000 -0.000000 6.607188

13 C -0.000000 0.000002 -0.000000 0.000000 -0.000000 -0.074993

14 C -0.000000 0.000003 -0.000000 -0.000000 0.000000 0.004175

15 C -0.000005 0.000168 -0.000051 -0.000000 -0.000000 -0.001735

16 N 0.000168 -0.003506 0.000222 0.000002 0.000003 -0.087484

17 C -0.000051 0.000222 -0.000012 -0.000000 -0.000000 0.605237

18 N -0.000001 -0.000003 -0.000023 -0.000000 -0.000000 -0.000152

19 N 0.000539 -0.020616 -0.003533 -0.000186 -0.000193 -0.000005

20 C -0.000003 0.000238 -0.000705 0.000019 -0.000003 -0.000031

21 C -0.000003 -0.000100 0.000082 0.000015 0.000000 -0.000000

22 C 0.000019 0.000375 0.003504 -0.000340 0.000010 -0.000000

23 C -0.001292 -0.003425 -0.097469 0.005460 -0.000270 -0.000001

24 N -0.001735 -0.087484 0.605237 -0.074993 0.004175 0.000000

25 Zn -0.016783 0.120058 -0.017791 -0.000492 -0.000481 -0.005340

26 C -0.000210 0.000064 0.000001 -0.000000 -0.000046 -0.000026

27 H 0.000009 0.000001 0.000000 0.000000 -0.000000 0.006079

28 C 0.009755 0.009125 -0.066597 0.263195 -0.056362 -0.000000

29 H -0.047385 0.006098 0.009774 -0.043139 0.394127 0.000000

30 C 0.000000 -0.000000 0.000000 -0.000000 -0.000000 0.014940

31 H 0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000005

32 C 0.000000 0.000001 0.000001 -0.000000 0.000000 0.000000

33 H 0.000001 0.000076 -0.000019 -0.000155 -0.000005 -0.000000

34 H 0.000042 0.000000 0.000000 0.000000 -0.000001 -0.000011

35 H 0.000041 0.000012 0.000000 0.000000 -0.000026 0.000006

36 H 0.000041 0.000012 0.000000 0.000000 -0.000026 0.000006

37 H -0.000129 0.000429 -0.004343 -0.044782 -0.000798 -0.000000

38 H -0.000129 0.000429 -0.004343 -0.044782 -0.000798 -0.000000

39 H 0.000182 -0.000243 0.006026 -0.040617 -0.005285 -0.000000

40 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.004512

41 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.004512

42 H 0.000000 -0.000000 0.000000 0.000000 0.000000 0.000094

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 0.005460 -0.000270 -0.001292 -0.003425 -0.097469 -0.000025

2 N -0.000186 -0.000193 0.000539 -0.020616 -0.003533 -0.000005

3 C 0.000019 -0.000003 -0.000003 0.000238 -0.000705 -0.000001

4 C 0.000015 0.000000 -0.000003 -0.000100 0.000082 -0.000000

5 C -0.000340 0.000010 0.000019 0.000375 0.003504 -0.000000

6 N -0.000000 -0.000000 -0.000001 -0.000003 -0.000023 0.000000

7 C -0.000000 -0.000000 -0.000005 0.000168 -0.000051 -0.000001

8 N 0.000002 0.000003 0.000168 -0.003506 0.000222 -0.000003

9 C -0.000000 -0.000000 -0.000051 0.000222 -0.000012 -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 -0.074993 0.004175 -0.001735 -0.087484 0.605237 -0.000152

13 C 5.058232 0.641035 -0.051652 -0.061284 0.367689 0.002921

14 C 0.641035 5.120709 0.388237 -0.096878 -0.065520 -0.043009

15 C -0.051652 0.388237 4.572749 0.397472 -0.123055 0.557075

16 N -0.061284 -0.096878 0.397472 7.174850 0.375430 -0.080548

17 C 0.367689 -0.065520 -0.123055 0.375430 4.607820 0.000579

18 N 0.002921 -0.043009 0.557075 -0.080548 0.000579 6.615756

19 N -0.000082 0.000166 -0.002802 -0.020555 0.000426 -0.076898

20 C 0.000073 0.004800 -0.095379 -0.004265 -0.001071 0.513358

21 C 0.000016 -0.000279 0.003234 -0.000051 0.000016 -0.078321

22 C 0.000000 0.000011 -0.000411 -0.000208 -0.000003 0.005152

23 C -0.000003 0.000018 -0.000893 0.000416 -0.000002 -0.001110

24 N -0.000000 -0.000000 -0.000016 -0.000003 -0.000001 -0.000140

25 Zn -0.000492 -0.000481 -0.016783 0.120058 -0.017791 -0.005424

26 C -0.000000 0.000000 0.000000 0.000001 0.000001 -0.000000

27 H -0.000155 -0.000005 0.000001 0.000076 -0.000019 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 0.263195 -0.056362 0.009755 0.009125 -0.066597 -0.000019

31 H -0.043139 0.394127 -0.047385 0.006098 0.009774 0.006832

32 C -0.000000 -0.000046 -0.000210 0.000064 0.000001 0.014466

33 H 0.000000 -0.000000 0.000009 0.000001 0.000000 -0.000016

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 -0.044782 -0.000798 -0.000129 0.000429 -0.004343 0.000010

41 H -0.044782 -0.000798 -0.000129 0.000429 -0.004343 0.000010

42 H -0.040617 -0.005285 0.000182 -0.000243 0.006026 -0.000010

43 H 0.000000 -0.000026 0.000041 0.000012 0.000000 0.004378

44 H 0.000000 -0.000026 0.000041 0.000012 0.000000 0.004378

45 H 0.000000 -0.000001 0.000042 0.000000 0.000000 0.000090

19 20 21 22 23 24

1 C 0.000154 -0.000046 -0.000000 -0.000000 -0.000006 -0.000001

2 N -0.003150 0.000214 0.000002 0.000003 0.000154 -0.000005

3 C 0.000214 -0.000014 -0.000000 -0.000000 -0.000046 -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 -0.000005 -0.000001 -0.000000 -0.000000 -0.000025 -0.000152

7 C 0.000539 -0.000003 -0.000003 0.000019 -0.001292 -0.001735

8 N -0.020616 0.000238 -0.000100 0.000375 -0.003425 -0.087484

9 C -0.003533 -0.000705 0.000082 0.003504 -0.097469 0.605237

10 C -0.000186 0.000019 0.000015 -0.000340 0.005460 -0.074993

11 C -0.000193 -0.000003 0.000000 0.000010 -0.000270 0.004175

12 N -0.000005 -0.000031 -0.000000 -0.000000 -0.000001 0.000000

13 C -0.000082 0.000073 0.000016 0.000000 -0.000003 -0.000000

14 C 0.000166 0.004800 -0.000279 0.000011 0.000018 -0.000000

15 C -0.002802 -0.095379 0.003234 -0.000411 -0.000893 -0.000016

16 N -0.020555 -0.004265 -0.000051 -0.000208 0.000416 -0.000003

17 C 0.000426 -0.001071 0.000016 -0.000003 -0.000002 -0.000001

18 N -0.076898 0.513358 -0.078321 0.005152 -0.001110 -0.000140

19 N 7.103763 0.388418 -0.066013 -0.097230 0.401444 -0.069642

20 C 0.388418 4.679180 0.427061 -0.072537 -0.137108 0.000871

21 C -0.066013 0.427061 5.066337 0.600926 -0.056288 0.004231

22 C -0.097230 -0.072537 0.600926 5.137975 0.443544 -0.045532

23 C 0.401444 -0.137108 -0.056288 0.443544 4.656557 0.467184

24 N -0.069642 0.000871 0.004231 -0.045532 0.467184 6.607188

25 Zn 0.117257 -0.017474 -0.000715 -0.000536 -0.016268 -0.005340

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 0.000062 0.000000 -0.000000 -0.000035 -0.000615 0.014940

29 H 0.000001 0.000000 0.000000 -0.000000 0.000014 -0.000005

30 C 0.000000 0.000003 -0.000000 0.000000 0.000000 -0.000000

31 H 0.000075 -0.000226 -0.000155 -0.000004 0.000001 0.000000

32 C 0.009105 -0.071206 0.267360 -0.055781 0.009545 -0.000026

33 H 0.006416 0.009685 -0.043748 0.397359 -0.050019 0.006079

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 -0.000023 -0.000108 0.004512

38 H 0.000015 -0.000000 0.000000 -0.000023 -0.000108 0.004512

39 H 0.000000 0.000000 0.000000 -0.000001 0.000041 0.000094

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 0.000424 -0.005778 -0.045436 -0.000040 -0.000085 0.000006

44 H 0.000424 -0.005778 -0.045436 -0.000040 -0.000085 0.000006

45 H -0.000238 0.006230 -0.041580 -0.005423 0.000220 -0.000011

25 26 27 28 29 30

1 C -0.016268 0.009545 -0.050019 0.000000 0.000001 -0.000615

2 N 0.117257 0.009105 0.006416 0.000000 0.000075 0.000062

3 C -0.017474 -0.071206 0.009685 0.000003 -0.000226 0.000000

4 C -0.000715 0.267360 -0.043748 -0.000000 -0.000155 -0.000000

5 C -0.000536 -0.055781 0.397359 0.000000 -0.000004 -0.000035

6 N -0.005424 0.014466 -0.000016 -0.000019 0.006832 0.000000

7 C -0.016783 -0.000210 0.000009 0.009755 -0.047385 0.000000

8 N 0.120058 0.000064 0.000001 0.009125 0.006098 -0.000000

9 C -0.017791 0.000001 0.000000 -0.066597 0.009774 0.000000

10 C -0.000492 -0.000000 0.000000 0.263195 -0.043139 -0.000000

11 C -0.000481 -0.000046 -0.000000 -0.056362 0.394127 -0.000000

12 N -0.005340 -0.000026 0.006079 -0.000000 0.000000 0.014940

13 C -0.000492 -0.000000 -0.000155 -0.000000 -0.000000 0.263195

14 C -0.000481 0.000000 -0.000005 -0.000000 -0.000000 -0.056362

15 C -0.016783 0.000000 0.000001 0.000000 0.000000 0.009755

16 N 0.120058 0.000001 0.000076 -0.000000 0.000000 0.009125

17 C -0.017791 0.000001 -0.000019 0.000000 -0.000000 -0.066597

18 N -0.005424 -0.000000 0.000000 0.000000 -0.000000 -0.000019

19 N 0.117257 -0.000000 0.000000 0.000062 0.000001 0.000000

20 C -0.017474 0.000000 -0.000000 0.000000 0.000000 0.000003

21 C -0.000715 -0.000000 -0.000000 -0.000000 0.000000 -0.000000

22 C -0.000536 -0.000000 -0.000000 -0.000035 -0.000000 0.000000

23 C -0.016268 0.000000 -0.000000 -0.000615 0.000014 0.000000

24 N -0.005340 0.000000 -0.000000 0.014940 -0.000005 -0.000000

25 Zn 10.223753 0.000404 -0.000034 0.000395 -0.000015 0.000395

26 C 0.000404 5.367701 -0.004361 -0.000000 0.000071 -0.000000

27 H -0.000034 -0.004361 0.453794 -0.000000 -0.000000 0.000070

28 C 0.000395 -0.000000 -0.000000 5.366890 -0.004801 0.000000

29 H -0.000015 0.000071 -0.000000 -0.004801 0.444952 -0.000000

30 C 0.000395 -0.000000 0.000070 0.000000 -0.000000 5.366890

31 H -0.000015 -0.000000 -0.000000 -0.000000 0.000000 -0.004801

32 C 0.000404 0.000000 -0.000000 -0.000000 -0.000000 -0.000000

33 H -0.000034 -0.000000 0.000000 0.000070 -0.000000 -0.000000

34 H 0.000071 0.389494 0.001421 -0.000000 0.000000 -0.000000

35 H 0.000080 0.388725 -0.000128 -0.000000 0.000040 0.000000

36 H 0.000080 0.388725 -0.000128 -0.000000 0.000040 0.000000

37 H 0.000076 0.000000 0.000000 0.388133 -0.000121 0.000000

38 H 0.000076 0.000000 0.000000 0.388133 -0.000121 0.000000

39 H 0.000070 -0.000000 0.000000 0.388985 0.001283 -0.000000

40 H 0.000076 -0.000000 0.000040 0.000000 -0.000000 0.388133

41 H 0.000076 -0.000000 0.000040 0.000000 -0.000000 0.388133

42 H 0.000070 -0.000000 0.000000 -0.000000 -0.000000 0.388985

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 0.000071 -0.000000 -0.000000 -0.000000 0.000000 -0.000000

31 32 33 34 35 36

1 C 0.000014 0.000000 -0.000000 0.000220 -0.000085 -0.000085

2 N 0.000001 -0.000000 0.000000 -0.000238 0.000424 0.000424

3 C 0.000000 0.000000 -0.000000 0.006230 -0.005778 -0.005778

4 C 0.000000 -0.000000 -0.000000 -0.041580 -0.045436 -0.045436

5 C -0.000000 -0.000000 -0.000000 -0.005423 -0.000040 -0.000040

6 N -0.000000 -0.000000 0.000000 0.000090 0.004378 0.004378

7 C 0.000000 0.000000 0.000001 0.000042 0.000041 0.000041

8 N 0.000000 0.000001 0.000076 0.000000 0.000012 0.000012

9 C -0.000000 0.000001 -0.000019 0.000000 0.000000 0.000000

10 C -0.000000 -0.000000 -0.000155 0.000000 0.000000 0.000000

11 C -0.000000 0.000000 -0.000005 -0.000001 -0.000026 -0.000026

12 N -0.000005 0.000000 -0.000000 -0.000011 0.000006 0.000006

13 C -0.043139 -0.000000 0.000000 0.000000 0.000000 0.000000

14 C 0.394127 -0.000046 -0.000000 0.000000 -0.000000 -0.000000

15 C -0.047385 -0.000210 0.000009 -0.000000 -0.000000 -0.000000

16 N 0.006098 0.000064 0.000001 -0.000000 0.000000 0.000000

17 C 0.009774 0.000001 0.000000 0.000001 -0.000000 -0.000000

18 N 0.006832 0.014466 -0.000016 -0.000000 -0.000000 -0.000000

19 N 0.000075 0.009105 0.006416 -0.000000 0.000000 0.000000

20 C -0.000226 -0.071206 0.009685 0.000000 0.000000 0.000000

21 C -0.000155 0.267360 -0.043748 0.000000 0.000000 0.000000

22 C -0.000004 -0.055781 0.397359 0.000000 -0.000000 -0.000000

23 C 0.000001 0.009545 -0.050019 0.000000 -0.000000 -0.000000

24 N 0.000000 -0.000026 0.006079 0.000000 0.000000 0.000000

25 Zn -0.000015 0.000404 -0.000034 0.000071 0.000080 0.000080

26 C -0.000000 0.000000 -0.000000 0.389494 0.388725 0.388725

27 H -0.000000 -0.000000 0.000000 0.001421 -0.000128 -0.000128

28 C -0.000000 -0.000000 0.000070 -0.000000 -0.000000 -0.000000

29 H 0.000000 -0.000000 -0.000000 0.000000 0.000040 0.000040

30 C -0.004801 -0.000000 -0.000000 -0.000000 0.000000 0.000000

31 H 0.444952 0.000071 -0.000000 0.000000 0.000000 0.000000

32 C 0.000071 5.367701 -0.004361 -0.000000 0.000000 0.000000

33 H -0.000000 -0.004361 0.453794 -0.000000 -0.000000 -0.000000

34 H 0.000000 -0.000000 -0.000000 0.461942 -0.025789 -0.025789

35 H 0.000000 0.000000 -0.000000 -0.025789 0.477280 -0.031553

36 H 0.000000 0.000000 -0.000000 -0.025789 -0.031553 0.477280

37 H -0.000000 -0.000000 0.000040 0.000000 0.000000 -0.000000

38 H -0.000000 -0.000000 0.000040 0.000000 -0.000000 0.000000

39 H -0.000000 -0.000000 0.000000 -0.000000 -0.000000 -0.000000

40 H -0.000121 0.000000 0.000000 -0.000000 -0.000000 0.000000

41 H -0.000121 0.000000 0.000000 -0.000000 0.000000 -0.000000

42 H 0.001283 -0.000000 0.000000 -0.000000 0.000000 0.000000

43 H 0.000040 0.388725 -0.000128 0.000000 -0.000000 0.000000

44 H 0.000040 0.388725 -0.000128 0.000000 0.000000 -0.000000

45 H 0.000000 0.389494 0.001421 0.000000 0.000000 0.000000

37 38 39 40 41 42

1 C 0.000000 0.000000 -0.000000 -0.000108 -0.000108 0.000041

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 -0.000023 -0.000023 -0.000001

6 N 0.000010 0.000010 -0.000010 0.000000 0.000000 0.000000

7 C -0.000129 -0.000129 0.000182 0.000000 0.000000 0.000000

8 N 0.000429 0.000429 -0.000243 0.000000 0.000000 -0.000000

9 C -0.004343 -0.004343 0.006026 0.000000 0.000000 0.000000

10 C -0.044782 -0.044782 -0.040617 0.000000 0.000000 0.000000

11 C -0.000798 -0.000798 -0.005285 0.000000 0.000000 0.000000

12 N -0.000000 -0.000000 -0.000000 0.004512 0.004512 0.000094

13 C 0.000000 0.000000 0.000000 -0.044782 -0.044782 -0.040617

14 C 0.000000 0.000000 0.000000 -0.000798 -0.000798 -0.005285

15 C 0.000000 0.000000 0.000000 -0.000129 -0.000129 0.000182

16 N 0.000000 0.000000 -0.000000 0.000429 0.000429 -0.000243

17 C 0.000000 0.000000 0.000000 -0.004343 -0.004343 0.006026

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 -0.000023 -0.000023 -0.000001 -0.000000 -0.000000 0.000000

23 C -0.000108 -0.000108 0.000041 0.000000 0.000000 -0.000000

24 N 0.004512 0.004512 0.000094 -0.000000 -0.000000 -0.000000

25 Zn 0.000076 0.000076 0.000070 0.000076 0.000076 0.000070

26 C 0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000000

27 H 0.000000 0.000000 0.000000 0.000040 0.000040 0.000000

28 C 0.388133 0.388133 0.388985 0.000000 0.000000 -0.000000

29 H -0.000121 -0.000121 0.001283 -0.000000 -0.000000 -0.000000

30 C 0.000000 0.000000 -0.000000 0.388133 0.388133 0.388985

31 H -0.000000 -0.000000 -0.000000 -0.000121 -0.000121 0.001283

32 C -0.000000 -0.000000 -0.000000 0.000000 0.000000 -0.000000

33 H 0.000040 0.000040 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 0.468205 -0.029445 -0.024937 -0.000000 0.000000 0.000000

38 H -0.029445 0.468205 -0.024937 0.000000 -0.000000 0.000000

39 H -0.024937 -0.024937 0.456377 0.000000 0.000000 0.000000

40 H -0.000000 0.000000 0.000000 0.468205 -0.029445 -0.024937

41 H 0.000000 -0.000000 0.000000 -0.029445 0.468205 -0.024937

42 H 0.000000 0.000000 0.000000 -0.024937 -0.024937 0.456377

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 -0.000026 -0.000026 -0.000001

15 C 0.000041 0.000041 0.000042

16 N 0.000012 0.000012 0.000000

17 C 0.000000 0.000000 0.000000

18 N 0.004378 0.004378 0.000090

19 N 0.000424 0.000424 -0.000238

20 C -0.005778 -0.005778 0.006230

21 C -0.045436 -0.045436 -0.041580

22 C -0.000040 -0.000040 -0.005423

23 C -0.000085 -0.000085 0.000220

24 N 0.000006 0.000006 -0.000011

25 Zn 0.000080 0.000080 0.000071

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 0.000040 0.000040 0.000000

32 C 0.388725 0.388725 0.389494

33 H -0.000128 -0.000128 0.001421

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 0.477280 -0.031553 -0.025789

44 H -0.031553 0.477280 -0.025789

45 H -0.025789 -0.025789 0.461942

Atomic-Atomic Spin Densities.

1 2 3 4 5 6

1 C 0.342573 0.007460 -0.025470 -0.023776 0.048397 0.000989

2 N 0.007460 -0.095062 0.000293 -0.003501 -0.000350 0.001741

3 C -0.025470 0.000293 0.326952 0.060412 -0.017468 -0.038583

4 C -0.023776 -0.003501 0.060412 0.159105 -0.039260 -0.005665

5 C 0.048397 -0.000350 -0.017468 -0.039260 0.023374 0.000279

6 N 0.000989 0.001741 -0.038583 -0.005665 0.000279 0.029276

7 C 0.000256 0.000247 -0.015581 -0.000797 0.000068 0.021327

8 N -0.000120 0.000158 0.002332 0.000046 -0.000009 -0.003390

9 C -0.000002 0.000024 0.000059 0.000000 -0.000000 0.000369

10 C -0.000000 -0.000002 0.000089 0.000000 -0.000000 -0.000287

11 C -0.000001 -0.000006 -0.000079 0.000032 -0.000000 -0.001486

12 N -0.034424 0.001088 0.000795 0.000482 -0.003749 -0.000002

13 C -0.000111 -0.000015 0.000000 -0.000000 0.000030 0.000000

14 C 0.000081 0.000001 -0.000000 -0.000000 -0.000000 0.000000

15 C 0.000060 0.000033 -0.000003 -0.000000 -0.000001 -0.000000

16 N 0.002481 0.000243 -0.000132 -0.000013 0.000046 0.000003

17 C -0.016672 -0.000211 0.000283 0.000101 -0.000643 -0.000002

18 N -0.000004 -0.000001 0.000000 0.000000 -0.000000 -0.000000

19 N 0.000002 -0.000003 0.000001 -0.000000 -0.000000 -0.000001

20 C -0.000001 0.000001 -0.000000 -0.000000 0.000000 0.000000

21 C 0.000000 -0.000000 -0.000000 -0.000000 0.000000 0.000000

22 C -0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000000

23 C -0.000000 0.000002 -0.000001 0.000000 -0.000000 -0.000004

24 N 0.000000 -0.000000 -0.000004 -0.000000 0.000000 0.000007

25 Zn 0.000291 0.001461 -0.000458 -0.000142 -0.000059 0.000059

26 C -0.000147 0.000001 -0.002052 -0.007397 0.003002 0.000602

27 H 0.000192 -0.000052 -0.000254 0.000550 0.000702 -0.000004

28 C 0.000000 -0.000000 0.000000 -0.000000 -0.000000 0.000000

29 H -0.000000 0.000000 -0.000019 0.000002 0.000000 0.000105

30 C 0.000011 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 0.000016 -0.000001 0.000056 -0.000426 0.000031 -0.000005

35 H 0.000090 0.000014 -0.001390 -0.003726 0.000458 0.000356

36 H 0.000090 0.000014 -0.001390 -0.003726 0.000458 0.000356

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 -0.000027 0.000000 0.000000 0.000000 -0.000004 -0.000000

41 H -0.000027 0.000000 0.000000 0.000000 -0.000004 -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 0.000256 -0.000120 -0.000002 -0.000000 -0.000001 -0.034424

2 N 0.000247 0.000158 0.000024 -0.000002 -0.000006 0.001088

3 C -0.015581 0.002332 0.000059 0.000089 -0.000079 0.000795

4 C -0.000797 0.000046 0.000000 0.000000 0.000032 0.000482

5 C 0.000068 -0.000009 -0.000000 -0.000000 -0.000000 -0.003749

6 N 0.021327 -0.003390 0.000369 -0.000287 -0.001486 -0.000002

7 C 0.146025 -0.013050 -0.007394 -0.007206 0.009001 -0.000001

8 N -0.013050 0.069262 -0.017214 0.001228 0.002656 0.000003

9 C -0.007394 -0.017214 0.157553 0.013339 -0.005782 -0.000000

10 C -0.007206 0.001228 0.013339 0.034371 -0.003421 0.000000

11 C 0.009001 0.002656 -0.005782 -0.003421 -0.006062 0.000000

12 N -0.000001 0.000003 -0.000000 0.000000 0.000000 0.011545

13 C -0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.001830

14 C 0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000421

15 C 0.000001 0.000006 -0.000008 -0.000000 0.000000 0.000427

16 N 0.000006 -0.000055 0.000005 -0.000000 -0.000000 -0.002768

17 C -0.000008 0.000005 0.000001 0.000000 -0.000000 0.020272

18 N -0.000000 0.000003 -0.000002 0.000000 0.000000 0.000007

19 N 0.000033 0.000243 -0.000211 -0.000015 0.000001 -0.000000

20 C -0.000003 -0.000132 0.000283 0.000000 -0.000000 -0.000004

21 C -0.000000 -0.000013 0.000101 -0.000000 -0.000000 -0.000000

22 C -0.000001 0.000046 -0.000643 0.000030 -0.000000 0.000000

23 C 0.000060 0.002481 -0.016672 -0.000111 0.000081 0.000000

24 N 0.000427 -0.002768 0.020272 -0.001830 -0.000421 -0.000000

25 Zn 0.000233 -0.001017 -0.000411 -0.000053 0.000044 0.000041

26 C 0.000055 0.000000 -0.000000 0.000000 -0.000002 -0.000000

27 H -0.000000 -0.000000 -0.000000 -0.000000 0.000000 0.000070

28 C -0.000047 0.000012 -0.001038 -0.001742 0.001145 0.000000

29 H 0.000139 -0.000027 -0.000083 0.000291 0.000247 0.000000

30 C 0.000000 -0.000000 -0.000000 0.000000 0.000000 0.000235

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 0.000001 -0.000011 -0.000000 0.000000 0.000000

34 H -0.000000 -0.000000 0.000000 -0.000000 0.000000 -0.000000

35 H 0.000060 -0.000002 0.000000 -0.000000 -0.000002 -0.000001

36 H 0.000060 -0.000002 0.000000 -0.000000 -0.000002 -0.000001

37 H 0.000030 -0.000031 -0.000130 -0.000987 -0.000012 -0.000000

38 H 0.000030 -0.000031 -0.000130 -0.000987 -0.000012 -0.000000

39 H 0.000012 0.000000 0.000032 -0.000107 -0.000008 -0.000000

40 H -0.000000 0.000000 -0.000000 0.000000 0.000000 0.000210

41 H -0.000000 0.000000 -0.000000 0.000000 0.000000 0.000210

42 H -0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.000005

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 -0.000111 0.000081 0.000060 0.002481 -0.016672 -0.000004

2 N -0.000015 0.000001 0.000033 0.000243 -0.000211 -0.000001

3 C 0.000000 -0.000000 -0.000003 -0.000132 0.000283 0.000000

4 C -0.000000 -0.000000 -0.000000 -0.000013 0.000101 0.000000

5 C 0.000030 -0.000000 -0.000001 0.000046 -0.000643 -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 -0.000008 -0.000000

8 N -0.000000 -0.000000 0.000006 -0.000055 0.000005 0.000003

9 C 0.000000 -0.000000 -0.000008 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 -0.001830 -0.000421 0.000427 -0.002768 0.020272 0.000007

13 C 0.034371 -0.003421 -0.007206 0.001228 0.013339 -0.000287

14 C -0.003421 -0.006062 0.009001 0.002656 -0.005782 -0.001486

15 C -0.007206 0.009001 0.146025 -0.013050 -0.007394 0.021327

16 N 0.001228 0.002656 -0.013050 0.069262 -0.017214 -0.003390

17 C 0.013339 -0.005782 -0.007394 -0.017214 0.157553 0.000369

18 N -0.000287 -0.001486 0.021327 -0.003390 0.000369 0.029276

19 N -0.000002 -0.000006 0.000247 0.000158 0.000024 0.001741

20 C 0.000089 -0.000079 -0.015581 0.002332 0.000059 -0.038583

21 C 0.000000 0.000032 -0.000797 0.000046 0.000000 -0.005665

22 C -0.000000 -0.000000 0.000068 -0.000009 -0.000000 0.000279

23 C -0.000000 -0.000001 0.000256 -0.000120 -0.000002 0.000989

24 N 0.000000 0.000000 -0.000001 0.000003 -0.000000 -0.000002

25 Zn -0.000053 0.000044 0.000233 -0.001017 -0.000411 0.000059

26 C 0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000000

27 H -0.000000 0.000000 -0.000000 0.000001 -0.000011 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 -0.001742 0.001145 -0.000047 0.000012 -0.001038 0.000000

31 H 0.000291 0.000247 0.000139 -0.000027 -0.000083 0.000105

32 C 0.000000 -0.000002 0.000055 0.000000 -0.000000 0.000602

33 H -0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000004

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 -0.000987 -0.000012 0.000030 -0.000031 -0.000130 0.000001

41 H -0.000987 -0.000012 0.000030 -0.000031 -0.000130 0.000001

42 H -0.000107 -0.000008 0.000012 0.000000 0.000032 -0.000000

43 H -0.000000 -0.000002 0.000060 -0.000002 0.000000 0.000356

44 H -0.000000 -0.000002 0.000060 -0.000002 0.000000 0.000356

45 H -0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.000005

19 20 21 22 23 24

1 C 0.000002 -0.000001 0.000000 -0.000000 -0.000000 0.000000

2 N -0.000003 0.000001 -0.000000 -0.000000 0.000002 -0.000000

3 C 0.000001 -0.000000 -0.000000 0.000000 -0.000001 -0.000004

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 -0.000001 0.000000 0.000000 -0.000000 -0.000004 0.000007

7 C 0.000033 -0.000003 -0.000000 -0.000001 0.000060 0.000427

8 N 0.000243 -0.000132 -0.000013 0.000046 0.002481 -0.002768

9 C -0.000211 0.000283 0.000101 -0.000643 -0.016672 0.020272

10 C -0.000015 0.000000 -0.000000 0.000030 -0.000111 -0.001830

11 C 0.000001 -0.000000 -0.000000 -0.000000 0.000081 -0.000421

12 N -0.000000 -0.000004 -0.000000 0.000000 0.000000 -0.000000

13 C -0.000002 0.000089 0.000000 -0.000000 -0.000000 0.000000

14 C -0.000006 -0.000079 0.000032 -0.000000 -0.000001 0.000000

15 C 0.000247 -0.015581 -0.000797 0.000068 0.000256 -0.000001

16 N 0.000158 0.002332 0.000046 -0.000009 -0.000120 0.000003

17 C 0.000024 0.000059 0.000000 -0.000000 -0.000002 -0.000000

18 N 0.001741 -0.038583 -0.005665 0.000279 0.000989 -0.000002

19 N -0.095062 0.000293 -0.003501 -0.000350 0.007460 0.001088

20 C 0.000293 0.326952 0.060412 -0.017468 -0.025470 0.000795

21 C -0.003501 0.060412 0.159105 -0.039260 -0.023776 0.000482

22 C -0.000350 -0.017468 -0.039260 0.023374 0.048397 -0.003749

23 C 0.007460 -0.025470 -0.023776 0.048397 0.342573 -0.034424

24 N 0.001088 0.000795 0.000482 -0.003749 -0.034424 0.011545

25 Zn 0.001461 -0.000458 -0.000142 -0.000059 0.000291 0.000041

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 0.000011 0.000235

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 0.000000 -0.000019 0.000002 0.000000 -0.000000 0.000000

32 C 0.000001 -0.002052 -0.007397 0.003002 -0.000147 -0.000000

33 H -0.000052 -0.000254 0.000550 0.000702 0.000192 0.000070

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 -0.000004 -0.000027 0.000210

38 H 0.000000 0.000000 0.000000 -0.000004 -0.000027 0.000210

39 H -0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000005

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 0.000014 -0.001390 -0.003726 0.000458 0.000090 -0.000001

44 H 0.000014 -0.001390 -0.003726 0.000458 0.000090 -0.000001

45 H -0.000001 0.000056 -0.000426 0.000031 0.000016 -0.000000

25 26 27 28 29 30

1 C 0.000291 -0.000147 0.000192 0.000000 -0.000000 0.000011

2 N 0.001461 0.000001 -0.000052 -0.000000 0.000000 0.000000

3 C -0.000458 -0.002052 -0.000254 0.000000 -0.000019 -0.000000

4 C -0.000142 -0.007397 0.000550 -0.000000 0.000002 0.000000

5 C -0.000059 0.003002 0.000702 -0.000000 0.000000 0.000002

6 N 0.000059 0.000602 -0.000004 0.000000 0.000105 0.000000

7 C 0.000233 0.000055 -0.000000 -0.000047 0.000139 0.000000

8 N -0.001017 0.000000 -0.000000 0.000012 -0.000027 -0.000000

9 C -0.000411 -0.000000 -0.000000 -0.001038 -0.000083 -0.000000

10 C -0.000053 0.000000 -0.000000 -0.001742 0.000291 0.000000

11 C 0.000044 -0.000002 0.000000 0.001145 0.000247 0.000000

12 N 0.000041 -0.000000 0.000070 0.000000 0.000000 0.000235

13 C -0.000053 0.000000 -0.000000 0.000000 0.000000 -0.001742

14 C 0.000044 -0.000000 0.000000 0.000000 0.000000 0.001145

15 C 0.000233 0.000000 -0.000000 0.000000 0.000000 -0.000047

16 N -0.001017 0.000000 0.000001 -0.000000 -0.000000 0.000012

17 C -0.000411 -0.000000 -0.000011 -0.000000 0.000000 -0.001038

18 N 0.000059 -0.000000 0.000000 0.000000 0.000000 0.000000

19 N 0.001461 0.000000 0.000000 0.000000 -0.000000 -0.000000

20 C -0.000458 0.000000 -0.000000 -0.000000 0.000000 0.000000

21 C -0.000142 0.000000 -0.000000 0.000000 -0.000000 -0.000000

22 C -0.000059 -0.000000 0.000000 0.000002 -0.000000 -0.000000

23 C 0.000291 -0.000000 0.000000 0.000011 0.000000 0.000000

24 N 0.000041 0.000000 0.000000 0.000235 -0.000003 0.000000

25 Zn -0.000661 -0.000007 -0.000000 -0.000007 -0.000001 -0.000007

26 C -0.000007 -0.012218 0.000348 0.000000 -0.000001 0.000000

27 H -0.000000 0.000348 -0.003768 -0.000000 0.000000 -0.000001

28 C -0.000007 0.000000 -0.000000 -0.002597 0.000127 0.000000

29 H -0.000001 -0.000001 0.000000 0.000127 -0.001129 -0.000000

30 C -0.000007 0.000000 -0.000001 0.000000 -0.000000 -0.002597

31 H -0.000001 -0.000000 0.000000 -0.000000 0.000000 0.000127

32 C -0.000007 0.000000 -0.000000 0.000000 -0.000000 0.000000

33 H -0.000000 -0.000000 0.000000 -0.000001 0.000000 -0.000000

34 H 0.000003 0.000762 -0.000078 -0.000000 0.000000 0.000000

35 H 0.000000 0.003516 0.000004 0.000000 -0.000001 0.000000

36 H 0.000000 0.003516 0.000004 0.000000 -0.000001 0.000000

37 H -0.000001 0.000000 -0.000000 0.000965 0.000002 0.000000

38 H -0.000001 0.000000 -0.000000 0.000965 0.000002 0.000000

39 H 0.000001 -0.000000 -0.000000 0.000216 -0.000031 0.000000

40 H -0.000001 0.000000 -0.000001 0.000000 -0.000000 0.000965

41 H -0.000001 0.000000 -0.000001 0.000000 -0.000000 0.000965

42 H 0.000001 0.000000 0.000000 0.000000 0.000000 0.000216

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 0.000003 -0.000000 0.000000 0.000000 -0.000000 -0.000000

31 32 33 34 35 36

1 C 0.000000 -0.000000 0.000000 0.000016 0.000090 0.000090

2 N -0.000000 0.000000 0.000000 -0.000001 0.000014 0.000014

3 C 0.000000 0.000000 -0.000000 0.000056 -0.001390 -0.001390

4 C -0.000000 0.000000 -0.000000 -0.000426 -0.003726 -0.003726

5 C -0.000000 -0.000000 0.000000 0.000031 0.000458 0.000458

6 N 0.000000 -0.000000 0.000000 -0.000005 0.000356 0.000356

7 C 0.000000 0.000000 -0.000000 -0.000000 0.000060 0.000060

8 N -0.000000 0.000000 0.000001 -0.000000 -0.000002 -0.000002

9 C 0.000000 -0.000000 -0.000011 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 -0.000002 -0.000002

12 N -0.000003 0.000000 0.000000 -0.000000 -0.000001 -0.000001

13 C 0.000291 0.000000 -0.000000 -0.000000 0.000000 0.000000

14 C 0.000247 -0.000002 0.000000 -0.000000 0.000000 0.000000

15 C 0.000139 0.000055 -0.000000 0.000000 0.000000 0.000000

16 N -0.000027 0.000000 -0.000000 0.000000 0.000000 0.000000

17 C -0.000083 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000

18 N 0.000105 0.000602 -0.000004 -0.000000 -0.000000 -0.000000

19 N 0.000000 0.000001 -0.000052 -0.000000 0.000000 0.000000

20 C -0.000019 -0.002052 -0.000254 -0.000000 0.000000 0.000000

21 C 0.000002 -0.007397 0.000550 -0.000000 0.000000 0.000000

22 C 0.000000 0.003002 0.000702 0.000000 -0.000000 -0.000000

23 C -0.000000 -0.000147 0.000192 0.000000 -0.000000 -0.000000

24 N 0.000000 -0.000000 0.000070 0.000000 0.000000 0.000000

25 Zn -0.000001 -0.000007 -0.000000 0.000003 0.000000 0.000000

26 C -0.000000 0.000000 -0.000000 0.000762 0.003516 0.003516

27 H 0.000000 -0.000000 0.000000 -0.000078 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 0.000127 0.000000 -0.000000 0.000000 0.000000 0.000000

31 H -0.001129 -0.000001 0.000000 -0.000000 0.000000 0.000000

32 C -0.000001 -0.012218 0.000348 -0.000000 -0.000000 -0.000000

33 H 0.000000 0.000348 -0.003768 0.000000 -0.000000 -0.000000

34 H -0.000000 -0.000000 0.000000 -0.000692 -0.000041 -0.000041

35 H 0.000000 -0.000000 -0.000000 -0.000041 0.011357 -0.003045

36 H 0.000000 -0.000000 -0.000000 -0.000041 -0.003045 0.011357

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 0.000002 0.000000 -0.000000 0.000000 -0.000000 0.000000

41 H 0.000002 0.000000 -0.000000 0.000000 0.000000 -0.000000

42 H -0.000031 -0.000000 -0.000000 -0.000000 0.000000 0.000000

43 H -0.000001 0.003516 0.000004 0.000000 -0.000000 0.000000

44 H -0.000001 0.003516 0.000004 0.000000 0.000000 -0.000000

45 H 0.000000 0.000762 -0.000078 -0.000000 0.000000 0.000000

37 38 39 40 41 42

1 C 0.000000 0.000000 0.000000 -0.000027 -0.000027 -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 -0.000004 -0.000004 0.000000

6 N 0.000001 0.000001 -0.000000 -0.000000 -0.000000 0.000000

7 C 0.000030 0.000030 0.000012 -0.000000 -0.000000 -0.000000

8 N -0.000031 -0.000031 0.000000 0.000000 0.000000 0.000000

9 C -0.000130 -0.000130 0.000032 -0.000000 -0.000000 -0.000000

10 C -0.000987 -0.000987 -0.000107 0.000000 0.000000 -0.000000

11 C -0.000012 -0.000012 -0.000008 0.000000 0.000000 0.000000

12 N -0.000000 -0.000000 -0.000000 0.000210 0.000210 -0.000005

13 C 0.000000 0.000000 -0.000000 -0.000987 -0.000987 -0.000107

14 C 0.000000 0.000000 0.000000 -0.000012 -0.000012 -0.000008

15 C -0.000000 -0.000000 -0.000000 0.000030 0.000030 0.000012

16 N 0.000000 0.000000 0.000000 -0.000031 -0.000031 0.000000

17 C -0.000000 -0.000000 -0.000000 -0.000130 -0.000130 0.000032

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 -0.000004 -0.000004 0.000000 0.000000 0.000000 -0.000000

23 C -0.000027 -0.000027 -0.000000 0.000000 0.000000 0.000000

24 N 0.000210 0.000210 -0.000005 -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 0.000965 0.000965 0.000216 0.000000 0.000000 0.000000

29 H 0.000002 0.000002 -0.000031 -0.000000 -0.000000 0.000000

30 C 0.000000 0.000000 0.000000 0.000965 0.000965 0.000216

31 H -0.000000 -0.000000 0.000000 0.000002 0.000002 -0.000031

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 0.003337 -0.000975 0.000003 -0.000000 0.000000 0.000000

38 H -0.000975 0.003337 0.000003 0.000000 -0.000000 0.000000

39 H 0.000003 0.000003 -0.000346 0.000000 0.000000 0.000000

40 H -0.000000 0.000000 0.000000 0.003337 -0.000975 0.000003

41 H 0.000000 -0.000000 0.000000 -0.000975 0.003337 0.000003

42 H 0.000000 0.000000 0.000000 0.000003 0.000003 -0.000346

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 -0.000002 -0.000002 0.000000

15 C 0.000060 0.000060 -0.000000

16 N -0.000002 -0.000002 -0.000000

17 C 0.000000 0.000000 0.000000

18 N 0.000356 0.000356 -0.000005

19 N 0.000014 0.000014 -0.000001

20 C -0.001390 -0.001390 0.000056

21 C -0.003726 -0.003726 -0.000426

22 C 0.000458 0.000458 0.000031

23 C 0.000090 0.000090 0.000016

24 N -0.000001 -0.000001 -0.000000

25 Zn 0.000000 0.000000 0.000003

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 0.003516 0.003516 0.000762

33 H 0.000004 0.000004 -0.000078

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 0.011357 -0.003045 -0.000041

44 H -0.003045 0.011357 -0.000041

45 H -0.000041 -0.000041 -0.000692

Mulliken charges and spin densities:

1 2

1 C 0.380629 0.302208

2 N -0.667774 -0.086424

3 C 0.381474 0.288386

4 C 0.008846 0.132301

5 C -0.310709 0.015300

6 N -0.439301 0.006044

7 C 0.412370 0.133981

8 N -0.706309 0.040618

9 C 0.407729 0.142307

10 C 0.023852 0.032597

11 C -0.283311 -0.004088

12 N -0.433918 -0.007828

13 C 0.023852 0.032597

14 C -0.283311 -0.004088

15 C 0.412370 0.133981

16 N -0.706309 0.040618

17 C 0.407729 0.142307

18 N -0.439301 0.006044

19 N -0.667774 -0.086424

20 C 0.381474 0.288386

21 C 0.008846 0.132301

22 C -0.310709 0.015300

23 C 0.380629 0.302208

24 N -0.433918 -0.007828

25 Zn 1.461819 -0.000713

26 C -0.704033 -0.010023

27 H 0.223621 -0.002299

28 C -0.701258 -0.001753

29 H 0.232664 -0.000380

30 C -0.701258 -0.001753

31 H 0.232664 -0.000380

32 C -0.704033 -0.010023

33 H 0.223621 -0.002299

34 H 0.239319 -0.000416

35 H 0.237849 0.007646

36 H 0.237849 0.007646

37 H 0.243266 0.002381

38 H 0.243266 0.002381

39 H 0.242969 -0.000230

40 H 0.243266 0.002381

41 H 0.243266 0.002381

42 H 0.242969 -0.000230

43 H 0.237849 0.007646

44 H 0.237849 0.007646

45 H 0.239319 -0.000416

Sum of Mulliken charges = -0.00000 2.00000

Mulliken charges and spin densities with hydrogens summed into heavy atoms:

1 2

1 C 0.380629 0.302208

2 N -0.667774 -0.086424

3 C 0.381474 0.288386

4 C 0.008846 0.132301

5 C -0.087089 0.013001

6 N -0.439301 0.006044

7 C 0.412370 0.133981

8 N -0.706309 0.040618

9 C 0.407729 0.142307

10 C 0.023852 0.032597

11 C -0.050647 -0.004469

12 N -0.433918 -0.007828

13 C 0.023852 0.032597

14 C -0.050647 -0.004469

15 C 0.412370 0.133981

16 N -0.706309 0.040618

17 C 0.407729 0.142307

18 N -0.439301 0.006044

19 N -0.667774 -0.086424

20 C 0.381474 0.288386

21 C 0.008846 0.132301

22 C -0.087089 0.013001

23 C 0.380629 0.302208

24 N -0.433918 -0.007828

25 Zn 1.461819 -0.000713

26 C 0.010984 0.004853

28 C 0.028244 0.002780

30 C 0.028244 0.002780

32 C 0.010984 0.004853

Electronic spatial extent (au): <R\*\*2>= 11217.9600

Charge= -0.0000 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= -166.6595 YY= -152.1654 ZZ= -172.0742

XY= -0.8204 XZ= -0.0000 YZ= -0.0000

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= -3.0264 YY= 11.4676 ZZ= -8.4412

XY= -0.8204 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= -6962.7096 YYYY= -6631.7509 ZZZZ= -206.9146 XXXY= 64.4929

XXXZ= -0.0000 YYYX= -100.5641 YYYZ= -0.0000 ZZZX= -0.0000

ZZZY= -0.0000 XXYY= -2633.5630 XXZZ= -1364.0987 YYZZ= -1354.1996

XXYZ= -0.0000 YYXZ= 0.0000 ZZXY= -0.7708

N-N= 2.761586671477D+03 E-N=-8.575129361013D+03 KE= 1.320804808098D+03

Symmetry AG KE= 6.508666445591D+02

Symmetry BG KE= 6.707690219656D+01

Symmetry AU KE= 2.107440598917D+01

Symmetry BU KE= 5.817868553537D+02

Isotropic Fermi Contact Couplings

Atom a.u. MegaHertz Gauss 10(-4) cm-1

1 C(13) 0.01967 11.05838 3.94591 3.68868

2 N(14) -0.01670 -2.69730 -0.96246 -0.89972

3 C(13) 0.01572 8.83433 3.15231 2.94682

4 C(13) 0.00037 0.20861 0.07444 0.06959

5 C(13) -0.00977 -5.48967 -1.95885 -1.83116

6 N(14) -0.00369 -0.59609 -0.21270 -0.19883

7 C(13) 0.00669 3.76312 1.34278 1.25524

8 N(14) 0.00218 0.35281 0.12589 0.11768

9 C(13) 0.00701 3.94053 1.40608 1.31442

10 C(13) -0.00200 -1.12434 -0.40119 -0.37504

11 C(13) -0.00480 -2.70008 -0.96346 -0.90065

12 N(14) -0.00514 -0.83070 -0.29641 -0.27709

13 C(13) -0.00200 -1.12434 -0.40119 -0.37504

14 C(13) -0.00480 -2.70008 -0.96346 -0.90065

15 C(13) 0.00669 3.76312 1.34278 1.25524

16 N(14) 0.00218 0.35281 0.12589 0.11768

17 C(13) 0.00701 3.94053 1.40608 1.31442

18 N(14) -0.00369 -0.59609 -0.21270 -0.19883

19 N(14) -0.01670 -2.69730 -0.96246 -0.89972

20 C(13) 0.01572 8.83433 3.15231 2.94682

21 C(13) 0.00037 0.20861 0.07444 0.06959

22 C(13) -0.00977 -5.48967 -1.95885 -1.83116

23 C(13) 0.01967 11.05838 3.94591 3.68868

24 N(14) -0.00514 -0.83070 -0.29641 -0.27709

25 Zn(67) 0.00000 0.00000 0.00000 0.00000

26 C(13) -0.00535 -3.00816 -1.07338 -1.00341

27 H(1) -0.00085 -1.90639 -0.68025 -0.63590

28 C(13) -0.00147 -0.82453 -0.29421 -0.27503

29 H(1) -0.00020 -0.45064 -0.16080 -0.15032

30 C(13) -0.00147 -0.82453 -0.29421 -0.27503

31 H(1) -0.00020 -0.45064 -0.16080 -0.15032

32 C(13) -0.00535 -3.00816 -1.07338 -1.00341

33 H(1) -0.00085 -1.90639 -0.68025 -0.63590

34 H(1) -0.00012 -0.27860 -0.09941 -0.09293

35 H(1) 0.00446 9.96126 3.55443 3.32272

36 H(1) 0.00446 9.96126 3.55443 3.32272

37 H(1) 0.00134 2.99787 1.06971 0.99998

38 H(1) 0.00134 2.99787 1.06971 0.99998

39 H(1) -0.00008 -0.18031 -0.06434 -0.06015

40 H(1) 0.00134 2.99787 1.06971 0.99998

41 H(1) 0.00134 2.99787 1.06971 0.99998

42 H(1) -0.00008 -0.18031 -0.06434 -0.06015

43 H(1) 0.00446 9.96126 3.55443 3.32272

44 H(1) 0.00446 9.96126 3.55443 3.32272

45 H(1) -0.00012 -0.27860 -0.09941 -0.09293

--------------------------------------------------------

Center ---- Spin Dipole Couplings ----

3XX-RR 3YY-RR 3ZZ-RR

--------------------------------------------------------

1 Atom -0.189082 -0.190242 0.379324

2 Atom 0.067061 0.071398 -0.138458

3 Atom -0.181068 -0.186012 0.367080

4 Atom -0.085168 -0.093764 0.178932

5 Atom -0.020242 -0.022571 0.042813

6 Atom -0.042603 -0.047260 0.089863

7 Atom -0.078617 -0.086662 0.165279

8 Atom -0.057729 -0.066609 0.124338

9 Atom -0.086186 -0.091268 0.177455

10 Atom -0.024331 -0.019713 0.044044

11 Atom -0.002646 -0.000357 0.003003

12 Atom -0.027478 -0.032540 0.060018

13 Atom -0.024331 -0.019713 0.044044

14 Atom -0.002646 -0.000357 0.003003

15 Atom -0.078617 -0.086662 0.165279

16 Atom -0.057729 -0.066609 0.124338

17 Atom -0.086186 -0.091268 0.177455

18 Atom -0.042603 -0.047260 0.089863

19 Atom 0.067061 0.071398 -0.138458

20 Atom -0.181068 -0.186012 0.367080

21 Atom -0.085168 -0.093764 0.178932

22 Atom -0.020242 -0.022571 0.042813

23 Atom -0.189082 -0.190242 0.379324

24 Atom -0.027478 -0.032540 0.060018

25 Atom -0.013339 0.016729 -0.003391

26 Atom 0.002629 -0.005974 0.003344

27 Atom 0.008226 -0.003550 -0.004676

28 Atom -0.003006 0.002275 0.000731

29 Atom -0.001499 0.004561 -0.003062

30 Atom -0.003006 0.002275 0.000731

31 Atom -0.001499 0.004561 -0.003062

32 Atom 0.002629 -0.005974 0.003344

33 Atom 0.008226 -0.003550 -0.004676

34 Atom 0.005000 -0.002315 -0.002685

35 Atom 0.002590 0.000217 -0.002808

36 Atom 0.002590 0.000217 -0.002808

37 Atom -0.000572 0.002487 -0.001915

38 Atom -0.000572 0.002487 -0.001915

39 Atom -0.001126 0.002715 -0.001589

40 Atom -0.000572 0.002487 -0.001915

41 Atom -0.000572 0.002487 -0.001915

42 Atom -0.001126 0.002715 -0.001589

43 Atom 0.002590 0.000217 -0.002808

44 Atom 0.002590 0.000217 -0.002808

45 Atom 0.005000 -0.002315 -0.002685

--------------------------------------------------------

XY XZ YZ

--------------------------------------------------------

1 Atom 0.004792 0.000000 0.000000

2 Atom 0.001053 -0.000000 -0.000000

3 Atom -0.006410 -0.000000 -0.000000

4 Atom 0.001953 0.000000 0.000000

5 Atom -0.002093 0.000000 0.000000

6 Atom -0.010274 -0.000000 0.000000

7 Atom -0.002095 0.000000 0.000000

8 Atom -0.000122 -0.000000 0.000000

9 Atom 0.002273 0.000000 -0.000000

10 Atom -0.001119 0.000000 -0.000000

11 Atom 0.000967 -0.000000 0.000000

12 Atom 0.010036 -0.000000 -0.000000

13 Atom -0.001119 0.000000 0.000000

14 Atom 0.000967 0.000000 -0.000000

15 Atom -0.002095 0.000000 0.000000

16 Atom -0.000122 -0.000000 -0.000000

17 Atom 0.002273 0.000000 0.000000

18 Atom -0.010274 -0.000000 -0.000000

19 Atom 0.001053 0.000000 0.000000

20 Atom -0.006410 -0.000000 0.000000

21 Atom 0.001953 -0.000000 -0.000000

22 Atom -0.002093 0.000000 0.000000

23 Atom 0.004792 -0.000000 -0.000000

24 Atom 0.010036 -0.000000 -0.000000

25 Atom -0.000488 -0.000000 -0.000000

26 Atom 0.003694 -0.000000 0.000000

27 Atom -0.005417 -0.000000 0.000000

28 Atom -0.001165 -0.000000 -0.000000

29 Atom 0.001088 0.000000 0.000000

30 Atom -0.001165 -0.000000 -0.000000

31 Atom 0.001088 -0.000000 0.000000

32 Atom 0.003694 0.000000 -0.000000

33 Atom -0.005417 0.000000 -0.000000

34 Atom 0.000925 -0.000000 -0.000000

35 Atom 0.003758 0.001789 0.002285

36 Atom 0.003758 -0.001789 -0.002285

37 Atom -0.001557 -0.000898 0.001123

38 Atom -0.001557 0.000898 -0.001123

39 Atom -0.000348 0.000000 0.000000

40 Atom -0.001557 0.000898 -0.001123

41 Atom -0.001557 -0.000898 0.001123

42 Atom -0.000348 0.000000 -0.000000

43 Atom 0.003758 -0.001789 -0.002285

44 Atom 0.003758 0.001789 0.002285

45 Atom 0.000925 -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 -0.1945 -26.099 -9.313 -8.706 -0.6632 0.7484 0.0000

1 C(13) Bbb -0.1848 -24.803 -8.850 -8.273 0.7484 0.6632 -0.0000

Bcc 0.3793 50.902 18.163 16.979 0.0000 0.0000 1.0000

Baa -0.1385 -5.340 -1.905 -1.781 0.0000 0.0000 1.0000

2 N(14) Bbb 0.0668 2.577 0.920 0.860 0.9746 -0.2241 0.0000

Bcc 0.0716 2.763 0.986 0.922 0.2241 0.9746 -0.0000

Baa -0.1904 -25.551 -9.117 -8.523 0.5658 0.8246 -0.0000

3 C(13) Bbb -0.1767 -23.707 -8.459 -7.908 0.8246 -0.5658 -0.0000

Bcc 0.3671 49.259 17.577 16.431 0.0000 0.0000 1.0000

Baa -0.0942 -12.639 -4.510 -4.216 -0.2117 0.9773 -0.0000

4 C(13) Bbb -0.0847 -11.372 -4.058 -3.793 0.9773 0.2117 -0.0000

Bcc 0.1789 24.011 8.568 8.009 0.0000 0.0000 1.0000

Baa -0.0238 -3.194 -1.140 -1.065 0.5068 0.8621 -0.0000

5 C(13) Bbb -0.0190 -2.551 -0.910 -0.851 0.8621 -0.5068 -0.0000

Bcc 0.0428 5.745 2.050 1.916 0.0000 0.0000 1.0000

Baa -0.0555 -2.139 -0.763 -0.714 0.6241 0.7814 -0.0000

6 N(14) Bbb -0.0344 -1.327 -0.473 -0.443 0.7814 -0.6241 0.0000

Bcc 0.0899 3.466 1.237 1.156 0.0000 0.0000 1.0000

Baa -0.0872 -11.698 -4.174 -3.902 0.2377 0.9713 -0.0000

7 C(13) Bbb -0.0781 -10.481 -3.740 -3.496 0.9713 -0.2377 0.0000

Bcc 0.1653 22.179 7.914 7.398 0.0000 0.0000 1.0000

Baa -0.0666 -2.569 -0.917 -0.857 0.0138 0.9999 -0.0000

8 N(14) Bbb -0.0577 -2.226 -0.794 -0.743 0.9999 -0.0138 0.0000

Bcc 0.1243 4.795 1.711 1.600 0.0000 0.0000 1.0000

Baa -0.0921 -12.364 -4.412 -4.124 -0.3568 0.9342 -0.0000

9 C(13) Bbb -0.0853 -11.449 -4.085 -3.819 0.9342 0.3568 -0.0000

Bcc 0.1775 23.813 8.497 7.943 0.0000 0.0000 1.0000

Baa -0.0246 -3.299 -1.177 -1.101 0.9747 0.2237 -0.0000

10 C(13) Bbb -0.0195 -2.611 -0.932 -0.871 -0.2237 0.9747 0.0000

Bcc 0.0440 5.910 2.109 1.971 0.0000 -0.0000 1.0000

Baa -0.0030 -0.403 -0.144 -0.134 0.9391 -0.3436 0.0000

11 C(13) Bbb -0.0000 -0.000 -0.000 -0.000 0.3436 0.9391 0.0000

Bcc 0.0030 0.403 0.144 0.134 -0.0000 0.0000 1.0000

Baa -0.0404 -1.557 -0.555 -0.519 -0.6146 0.7888 -0.0000

12 N(14) Bbb -0.0197 -0.758 -0.271 -0.253 0.7888 0.6146 -0.0000

Bcc 0.0600 2.315 0.826 0.772 0.0000 0.0000 1.0000

Baa -0.0246 -3.299 -1.177 -1.101 0.9747 0.2237 -0.0000

13 C(13) Bbb -0.0195 -2.611 -0.932 -0.871 -0.2237 0.9747 0.0000

Bcc 0.0440 5.910 2.109 1.971 0.0000 0.0000 1.0000

Baa -0.0030 -0.403 -0.144 -0.134 0.9391 -0.3436 0.0000

14 C(13) Bbb -0.0000 -0.000 -0.000 -0.000 0.3436 0.9391 0.0000

Bcc 0.0030 0.403 0.144 0.134 0.0000 0.0000 1.0000

Baa -0.0872 -11.698 -4.174 -3.902 0.2377 0.9713 -0.0000

15 C(13) Bbb -0.0781 -10.481 -3.740 -3.496 0.9713 -0.2377 -0.0000

Bcc 0.1653 22.179 7.914 7.398 0.0000 0.0000 1.0000

Baa -0.0666 -2.569 -0.917 -0.857 0.0138 0.9999 -0.0000

16 N(14) Bbb -0.0577 -2.226 -0.794 -0.743 0.9999 -0.0138 -0.0000

Bcc 0.1243 4.795 1.711 1.600 0.0000 0.0000 1.0000

Baa -0.0921 -12.364 -4.412 -4.124 -0.3568 0.9342 -0.0000

17 C(13) Bbb -0.0853 -11.449 -4.085 -3.819 0.9342 0.3568 -0.0000

Bcc 0.1775 23.813 8.497 7.943 0.0000 0.0000 1.0000

Baa -0.0555 -2.139 -0.763 -0.714 0.6241 0.7814 -0.0000

18 N(14) Bbb -0.0344 -1.327 -0.473 -0.443 0.7814 -0.6241 -0.0000

Bcc 0.0899 3.466 1.237 1.156 0.0000 0.0000 1.0000

Baa -0.1385 -5.340 -1.905 -1.781 0.0000 0.0000 1.0000

19 N(14) Bbb 0.0668 2.577 0.920 0.860 0.9746 -0.2241 0.0000

Bcc 0.0716 2.763 0.986 0.922 0.2241 0.9746 -0.0000

Baa -0.1904 -25.551 -9.117 -8.523 0.5658 0.8246 0.0000

20 C(13) Bbb -0.1767 -23.707 -8.459 -7.908 0.8246 -0.5658 -0.0000

Bcc 0.3671 49.259 17.577 16.431 0.0000 0.0000 1.0000

Baa -0.0942 -12.639 -4.510 -4.216 -0.2117 0.9773 -0.0000

21 C(13) Bbb -0.0847 -11.372 -4.058 -3.793 0.9773 0.2117 -0.0000

Bcc 0.1789 24.011 8.568 8.009 0.0000 0.0000 1.0000

Baa -0.0238 -3.194 -1.140 -1.065 0.5068 0.8621 -0.0000

22 C(13) Bbb -0.0190 -2.551 -0.910 -0.851 0.8621 -0.5068 0.0000

Bcc 0.0428 5.745 2.050 1.916 0.0000 0.0000 1.0000

Baa -0.1945 -26.099 -9.313 -8.706 -0.6632 0.7484 0.0000

23 C(13) Bbb -0.1848 -24.803 -8.850 -8.273 0.7484 0.6632 -0.0000

Bcc 0.3793 50.902 18.163 16.979 0.0000 0.0000 1.0000

Baa -0.0404 -1.557 -0.555 -0.519 -0.6146 0.7888 -0.0000

24 N(14) Bbb -0.0197 -0.758 -0.271 -0.253 0.7888 0.6146 0.0000

Bcc 0.0600 2.315 0.826 0.772 0.0000 0.0000 1.0000

Baa -0.0133 -0.446 -0.159 -0.149 0.9999 0.0162 0.0000

25 Zn(67) Bbb -0.0034 -0.113 -0.040 -0.038 0.0000 0.0000 1.0000

Bcc 0.0167 0.560 0.200 0.187 -0.0162 0.9999 -0.0000

Baa -0.0073 -0.985 -0.352 -0.329 -0.3474 0.9377 -0.0000

26 C(13) Bbb 0.0033 0.449 0.160 0.150 -0.0000 -0.0000 1.0000

Bcc 0.0040 0.537 0.191 0.179 0.9377 0.3474 0.0000

Baa -0.0057 -3.021 -1.078 -1.008 0.3633 0.9317 -0.0000

27 H(1) Bbb -0.0047 -2.495 -0.890 -0.832 0.0000 0.0000 1.0000

Bcc 0.0103 5.516 1.968 1.840 0.9317 -0.3633 0.0000

Baa -0.0033 -0.436 -0.156 -0.146 0.9785 0.2062 0.0000

28 C(13) Bbb 0.0007 0.098 0.035 0.033 -0.0000 -0.0000 1.0000

Bcc 0.0025 0.338 0.121 0.113 -0.2062 0.9785 0.0000

Baa -0.0031 -1.633 -0.583 -0.545 0.0000 0.0000 1.0000

29 H(1) Bbb -0.0017 -0.901 -0.321 -0.301 0.9852 -0.1715 0.0000

Bcc 0.0048 2.534 0.904 0.845 0.1715 0.9852 -0.0000

Baa -0.0033 -0.436 -0.156 -0.146 0.9785 0.2062 -0.0000

30 C(13) Bbb 0.0007 0.098 0.035 0.033 0.0000 0.0000 1.0000

Bcc 0.0025 0.338 0.121 0.113 -0.2062 0.9785 -0.0000

Baa -0.0031 -1.633 -0.583 -0.545 0.0000 0.0000 1.0000

31 H(1) Bbb -0.0017 -0.901 -0.321 -0.301 0.9852 -0.1715 -0.0000

Bcc 0.0048 2.534 0.904 0.845 0.1715 0.9852 0.0000

Baa -0.0073 -0.985 -0.352 -0.329 -0.3474 0.9377 0.0000

32 C(13) Bbb 0.0033 0.449 0.160 0.150 0.0000 0.0000 1.0000

Bcc 0.0040 0.537 0.191 0.179 0.9377 0.3474 -0.0000

Baa -0.0057 -3.021 -1.078 -1.008 0.3633 0.9317 0.0000

33 H(1) Bbb -0.0047 -2.495 -0.890 -0.832 0.0000 0.0000 1.0000

Bcc 0.0103 5.516 1.968 1.840 0.9317 -0.3633 0.0000

Baa -0.0027 -1.433 -0.511 -0.478 0.0000 0.0000 1.0000

34 H(1) Bbb -0.0024 -1.297 -0.463 -0.433 -0.1235 0.9923 -0.0000

Bcc 0.0051 2.729 0.974 0.910 0.9923 0.1235 -0.0000

Baa -0.0040 -2.159 -0.771 -0.720 0.0579 -0.5107 0.8578

35 H(1) Bbb -0.0022 -1.157 -0.413 -0.386 0.6545 -0.6294 -0.4189

Bcc 0.0062 3.317 1.183 1.106 0.7539 0.5857 0.2978

Baa -0.0040 -2.159 -0.771 -0.720 -0.0579 0.5107 0.8578

36 H(1) Bbb -0.0022 -1.157 -0.413 -0.386 0.6545 -0.6294 0.4189

Bcc 0.0062 3.317 1.183 1.106 0.7539 0.5857 -0.2978

Baa -0.0024 -1.277 -0.456 -0.426 0.3757 -0.0924 0.9221

37 H(1) Bbb -0.0011 -0.588 -0.210 -0.196 0.8390 0.4565 -0.2960

Bcc 0.0035 1.865 0.666 0.622 -0.3936 0.8849 0.2490

Baa -0.0024 -1.277 -0.456 -0.426 -0.3757 0.0924 0.9221

38 H(1) Bbb -0.0011 -0.588 -0.210 -0.196 0.8390 0.4565 0.2960

Bcc 0.0035 1.865 0.666 0.622 -0.3936 0.8849 -0.2490

Baa -0.0016 -0.848 -0.303 -0.283 -0.0000 -0.0000 1.0000

39 H(1) Bbb -0.0012 -0.617 -0.220 -0.206 0.9960 0.0895 0.0000

Bcc 0.0027 1.465 0.523 0.489 -0.0895 0.9960 0.0000

Baa -0.0024 -1.277 -0.456 -0.426 -0.3757 0.0924 0.9221

40 H(1) Bbb -0.0011 -0.588 -0.210 -0.196 0.8390 0.4565 0.2960

Bcc 0.0035 1.865 0.666 0.622 -0.3936 0.8849 -0.2490

Baa -0.0024 -1.277 -0.456 -0.426 0.3757 -0.0924 0.9221

41 H(1) Bbb -0.0011 -0.588 -0.210 -0.196 0.8390 0.4565 -0.2960

Bcc 0.0035 1.865 0.666 0.622 -0.3936 0.8849 0.2490

Baa -0.0016 -0.848 -0.303 -0.283 0.0000 0.0000 1.0000

42 H(1) Bbb -0.0012 -0.617 -0.220 -0.206 0.9960 0.0895 0.0000

Bcc 0.0027 1.465 0.523 0.489 -0.0895 0.9960 -0.0000

Baa -0.0040 -2.159 -0.771 -0.720 -0.0579 0.5107 0.8578

43 H(1) Bbb -0.0022 -1.157 -0.413 -0.386 0.6545 -0.6294 0.4189

Bcc 0.0062 3.317 1.183 1.106 0.7539 0.5857 -0.2978

Baa -0.0040 -2.159 -0.771 -0.720 0.0579 -0.5107 0.8578

44 H(1) Bbb -0.0022 -1.157 -0.413 -0.386 0.6545 -0.6294 -0.4189

Bcc 0.0062 3.317 1.183 1.106 0.7539 0.5857 0.2978

Baa -0.0027 -1.433 -0.511 -0.478 0.0000 -0.0000 1.0000

45 H(1) Bbb -0.0024 -1.297 -0.463 -0.433 -0.1235 0.9923 0.0000

Bcc 0.0051 2.729 0.974 0.910 0.9923 0.1235 -0.0000

---------------------------------------------------------------------------------

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Tue Sep 17 14:42:39 2019, MaxMem= 2415919104 cpu: 29.2

(Enter /home/blab/g09/l9999.exe)

1\1\ WCSS.PL-BEM-DHCP-129-94-98-136\FOpt\UB3LYP\GenECP\C20H16N8Zn1(3)\

BLAB\17-Sep-2019\0\\#p opt=GDIIS b3lyp/genecp scrf=(solvent=dmso,smd)

empiricaldispersion=gd3bj\\ZntAzP3\\0,3\C,-2.0733148809,-2.1918408741,

0.\N,-0.7465894714,-1.8659191044,0.\C,-0.0069048831,-3.0024658971,0.\C

,-0.9175413189,-4.1534709755,0.\C,-2.189957046,-3.6330486699,0.\N,1.35

43256056,-3.1060040675,0.\C,2.1783653346,-2.07300043,0.\N,1.8573030017

,-0.7442627646,0.\C,2.9980668866,0.0037720007,0.\C,4.1701144898,-0.937

5774193,0.\C,3.6559087697,-2.1852324395,0.\N,-3.1238013201,-1.31430208

71,0.\C,-4.1701144898,0.9375774193,0.\C,-3.6559087697,2.1852324395,0.\

C,-2.1783653346,2.07300043,0.\N,-1.8573030017,0.7442627646,0.\C,-2.998

0668866,-0.0037720007,0.\N,-1.3543256056,3.1060040675,0.\N,0.746589471

4,1.8659191044,0.\C,0.0069048831,3.0024658971,0.\C,0.9175413189,4.1534

709755,0.\C,2.189957046,3.6330486699,0.\C,2.0733148809,2.1918408741,0.

\N,3.1238013201,1.3143020871,0.\Zn,0.,0.,0.\C,-0.4793412537,-5.5762416

113,0.\H,-3.1231016496,-4.1790164325,0.\C,5.5844696665,-0.4837202066,0

.\H,4.191364071,-3.1245543296,0.\C,-5.5844696665,0.4837202066,0.\H,-4.

191364071,3.1245543296,0.\C,0.4793412537,5.5762416114,0.\H,3.123101649

6,4.1790164325,0.\H,-1.3340610664,-6.2548588367,0.\H,0.1368859865,-5.8

005761773,0.8770796928\H,0.1368859865,-5.8005761773,-0.8770796928\H,5.

7933732104,0.1375409066,0.8768321227\H,5.7933732104,0.1375409066,-0.87

68321227\H,6.2746929011,-1.3285557867,0.\H,-5.7933732104,-0.1375409066

,0.8768321227\H,-5.7933732104,-0.1375409066,-0.8768321227\H,-6.2746929

011,1.3285557867,0.\H,-0.1368859865,5.8005761773,0.8770796928\H,-0.136

8859865,5.8005761773,-0.8770796928\H,1.3340610664,6.2548588367,0.\\Ver

sion=ES64L-G09RevE.01\State=3-BU\HF=-1275.842677\S2=2.017779\S2-1=0.\S

2A=2.000189\RMSD=4.259e-09\RMSF=8.530e-05\Dipole=0.,0.,0.\Quadrupole=7

.4560959,-1.1803023,-6.2757937,-3.2795529,0.,0.\PG=C02H [O(Zn1),SGH(C2

0H8N8),X(H8)]\\@

TO DETECT ERRORS, THE PROGRAMMER MUST HAVE A CONNIVING MIND,

ONE THAT DELIGHTS IN UNCOVERING FLAWS WHERE BEAUTY AND

PERFECTION WERE ONCE THOUGHT TO LIE.

-- THE PSYCHOLOGY OF COMPUTER PROGRAMMING

GERALD M. WEINBERG

Job cpu time: 0 days 16 hours 0 minutes 5.8 seconds.

File lengths (MBytes): RWF= 742 Int= 0 D2E= 0 Chk= 34 Scr= 1

Normal termination of Gaussian 09 at Tue Sep 17 14:42:39 2019.